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# Definition of Recommended Values of Certain Thermodynamic Properties for the Ketones

Thermodynamics Research Laboratory  
Box 1144  
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St. Louis, Missouri 63130

December 1983

Final Report to Office of Standard Reference Data, NBS

Issued January 1984



—QC— U.S. DEPARTMENT OF COMMERCE

100 NATIONAL BUREAU OF STANDARDS

U56

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**DEFINITION OF RECOMMENDED  
VALUES OF CERTAIN THERMODYNAMIC  
PROPERTIES FOR THE KETONES**

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Issued January 1984

**U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary  
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director**



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Definition of Recommended Values of Certain  
Thermodynamic Properties for the Ketones

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Experimental data for the vapor pressure, liquid density, second virial coefficient, and certain compound constants for the ketones were retrieved in a comprehensive sweep of the literature. The vapor pressure and liquid density data were subjected to an intensive selection-deletion process to identify the best available experimental data points for each compound. Those data were carefully correlated with reliable equations in order to put the selected data into a form convenient for use in computer data banks. The second virial coefficient data were not subjected to such an intensive evaluation process; that predictive correlation equation which provided the best overall representation of the literature data sets for each compound was chosen for use in the data bank. Values of the compound constants were selected subject to the requirement that those constants related to the vapor pressure and liquid density be consistent with the selected correlations for those properties. Whenever possible, the parameters for the best available equations of state are provided. The correlation equations can be used to provide tabulations of vapor pressure, saturated liquid density, second virial coefficients, heat of vaporization, and saturated vapor volume to the extent permitted by the available good experimental data.

Key words: Critical properties; data evaluation; equation of state; ketones; liquid density; literature retrieval; melting point; normal boiling point; property correlation; second virial coefficient; selected data; vapor pressure.

## 1. Scope of Project

### 1.1. Relevant Compounds

The compounds relevant to this report have the following three characteristics: (a) they contain only elements from the following list,

carbon

hydrogen

oxygen

nitrogen

sulfur

halogens (F, Cl, Br, I)

"rare" gases (He, Ne, Ar, Kr, Xe, Rn)

silicon,

(b) they contain one or more carbonyl ( $C=O$ ) groups, and (c) they contain only those other characteristic groups which fall below the carbonyl group in the IUPAC priority list for citation as the principal group. Those classes of compounds whose characteristic groups fall below the ketones are the alcohols, phenols, thiols, hydroperoxides, amines, imines, ethers, sulfides and peroxides. Those characteristic groups excluded by the IUPAC priority list are the carboxylic acid, sulfonic acid, ester, acid halide, amide, amidine, nitrile and aldehyde groups.

If a compound which satisfies the above criteria does not appear in this report, its absence is due to the fact that no useable data were found for that compound in the literature.

## 1.2. Properties Covered

An attempt has been made to report values of the following properties for all those relevant compounds for which useable data appear in the literature:

1. Compound constants (melting point, normal boiling point, critical properties and acentric factor).
2. Vapor pressure.
3. Saturated liquid density.
4. Second virial coefficient.

In addition, equation of state constants are tabulated whenever they are available.

Two calculated properties follow easily from the above experimental properties--the saturated vapor molar volume and the heat of vaporization--and those properties are included in the data tables whenever possible. When the vapor pressure is known and an adequate equation of state is available, the saturated vapor molar volume can be calculated. The heat of vaporization can be calculated from the Clapeyron equation when vapor pressure, saturated vapor molar volume and the saturated liquid molar volume are all available.

not at high  
P

Because of their usefulness in various correlations, particularly those for the second virial coefficient, values of the dipole moment and the radius of gyration also have been included when readily available. No attempt was made to retrieve and evaluate literature values for the dipole moment, nor to calculate values for the radius of gyration. The dipole moment values listed were taken from McClelland [5266]<sup>1</sup> and the radius of gyration values from Thompson [1706].

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<sup>1</sup>Figures in brackets indicate literature references listed in the References section at the end of this report.

### 1.3. Literature Covered

The ketone project was part of a long-range program dealing with all organic and some inorganic compounds. Over 25,000 relevant literature documents have been retrieved as part of the overall program, and it is believed that number is within 1000 to 2000 of the total number of relevant documents in existence. Retrieval of old documents is continuing along with the retrieval of newly-published relevant documents.

Literature searches for specific compounds are not feasible when retrieving on such a large scale. As an alternative, four techniques have been used in an attempt to sweep all the relevant documents from the published literature:

1. Selected journals (see table 1) have been "clean-swept"; i.e., a trained searcher leafed through the journal from the first to the last volume looking for relevant documents. The titles and abstracts were not assumed to be sufficient evidence of relevancy or non-relevancy.
2. About 100 compilations, bibliographies, review articles, etc., dealing with the compounds and properties of interest were searched for literature citations of interest.
3. The relevant sections in all the Chemical Abstract volumes for Volume 1 (1907) through Volume 64 (1965) were swept. After 1965, the yearly volumes of the Bulletin of Chemical Thermodynamics were substituted for Chemical Abstracts.
4. The literature citations in each document from which data are transcribed were checked for relevancy and the documents retrieved if not already in hand.

Table 1. Journals which have been clean-swept

---

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|  |
|--|
| Acta Chemica Scandinavica  |
| AICHE Journal  |
| Australian Journal of Chemistry                                      |
| Berichte der Bunsengesellschaft fuer Physikalische Chemie            |
| Canadian Journal of Chemistry  |
| Chemical Engineering Progress  |
| Chemical Engineering Progress, Symposium Series                      |
| Chemical Engineering Science   |
| Chemical Reviews   |
| Chemical Society Reviews   |
| Collection Czechoslovak Chemical Communications                      |
| Discussions of the Faraday Society                                   |
| Fluid Phase Equilibria   |
| Industrial and Engineering Chemistry                                 |
| Industrial and Engineering Chemistry, Fundamentals                   |
| Industrial and Engineering Chemistry, Process Design and Development |
| Journal of American Chemical Society                                 |
| Journal of Applied Chemistry (USSR)                                  |
| Journal of Chemical and Engineering Data                             |
| Journal of Chemical Physics  |
| Journal Chemical Society, Faraday Transactions I.                    |
| Journal Chemical Society, Faraday Transactions II.                   |
| Journal of Chemical Society (London)                                 |
| Journal of Chemical Thermodynamics                                   |
| Journal de Chimie Physique   |
| Journal fuer Praktische Chemie                                       |
| Journal Physical and Chemical Reference Data                         |
| Journal of Physical Chemistry  |
| Thermochimica Acta   |
| Pure and Applied Chemistry   |
| Russian Journal of Physical Chemistry                                |
| Transactions of the American Institute of Chemical Engineers         |
| Transactions of Faraday Society                                      |
| Zeitschrift fuer Physikalische Chemie (Frankfurt)                    |
| Zeitschrift fuer Physikalische Chemie (Leipzig)                      |

Newly-published relevant documents are identified by scanning the weekly issues of Current Contents/Physical Sciences, and by periodic updates of the first three items listed above.

One major omission in the coverage of the literature should be noted. No attempt was made to cover all the organic synthesis literature where melting point, boiling point, and 20° or 25 °C density data are often reported as a means of identification of a newly synthesized compound. There are two reasons for that omission. First, that body of literature is very large, and its coverage would have increased the retrieval load by at least another 10,000 documents. Second, the compound constant values reported are usually suspect because of uncertain purities, poor measurement techniques, etc. Hence, a very large expenditure of effort almost invariably yields very little in the way of useful results. Consequently, the decision was made to concentrate on those documents where the measurement of thermodynamic data was a primary objective of the authors.

It is believed that the above approach to retrieval makes available over 95% of all relevant documents and over 98% of the useable data. The overall retrieval percentage for the good data probably approaches 100% but it is always possible to miss an important document for a specific compound when dealing with hundreds of compounds and thousands of documents. The authors will appreciate being informed of any such omissions.

Of the 25,000+ documents which were retrieved, 2956 contained some sort of information on ketones. Of those 2956, only 784 reported data on properties relevant to this project.

## 2. Project Output

The objective of the long-range program, of which this ketone project has been a part, is the development of thermodynamic data banks which can be stored in the user's computer system. A strong effort is made to identify, retrieve and screen all the useable literature data for the properties covered. The selected literature data are then stored in the data bank, with the temperature-dependent properties being stored in the form of correlation constants. The data banks, plus their associated software, make all the useful literature data available to the user through his computer terminal in an immediately useful form. Or, the user may have his computer programs access the data banks directly for the needed thermodynamic data.

*irrelevant  
to this paper  
sounds like  
an id*

The emphasis upon computer accessibility has had a major impact upon the reporting format for this project. The selected values for the temperature dependent properties--vapor pressure, liquid density and second virial equation--are reported in the form of constants for correlation equations. For the user who needs the selected data values in readable form, tables can be generated over the temperature ranges corresponding to the experimental data limits on the correlating equations. Those tables also include two calculated properties--the saturated vapor molar volume and the heat of vaporization--whenever the data necessary for their calculation are available.

When numerical data values are processed en masse through a computer, it becomes difficult to reflect the reliability of a recommended value by the number of decimal digits carried, and the attempt to do so was finally abandoned. The number of digits printed was set to accommodate the best data --three decimal digits for temperature, six decimal digits for density, etc.-- and all property values printed with the same number of digits regardless of reliability. Hence, the reader must become accustomed to the sight of a normal boiling point printed with three decimal places when the uncertainty may be as high as 1 or 2 K in extreme cases. Or, the sight of density values printed with six decimal places when only three would be sufficient to carry all the information provided by the experimental measurements. The printing of the extra digits does have some justification beyond that of expediency when the units must be changed. Two unit conversion steps with truncation back to the number of justified digits after each conversion can sometimes create a result which, if it is then converted back to the original units, is quite different from the original literature value. That situation sometimes arises when authors have reported their results twice in different journals using different units. Then when the two sets of values are both converted to SI units and compared, the differences are uncomfortably large. The only way to minimize the effect of such numerical static is to minimize the effect of truncation by carrying extra digits.

The fact that the ketone project was a part of the larger data evaluation project influenced the reporting format in an additional way. As the literature documents are retrieved, their citations are added to the Laboratory's Master Reference List (MRL). The MRL number serves as a document's identification number in the data processing, and that method of identification has been retained in this report. The reader will note that the number sequence in the ketone bibliography in the References section is not continuous, but otherwise the MRL numbers which appear in this report are just like ordinary reference numbers.

### 3. Units

The conversion of the literature data to the units used for processing and reporting is accomplished by the CON programs (CONCON for compound constants, VAPCON for vapor pressure, DENCON for liquid density and BCON for the second virial coefficient). The conversion units used by the CON programs are given in the identity strings below. The first unit in each string is the unit used for processing.

$$1.0 \text{ K} = {}^\circ\text{C} + 273.15 = 273.15 + ({}^\circ\text{F}-32)/1.8 = {}^\circ\text{R}/1.8$$

$$\begin{aligned} 101.325 \text{ kPa} &= 1.0 \text{ atm} = 760 \text{ mm Hg} = 14.69595 \text{ psi} \\ &= 29.92126 \text{ in. Hg.} = 1.033227 \text{ kg/cm}^2 = 1.01325 \text{ bar} \end{aligned}$$

$$1.0 \text{ g/cm}^3 = 1.000028 \text{ g/ml(old)} = 62.42795 \text{ lb/ft}^3 = 8.345403 \text{ lb/gal}$$

The water density data of Kell [3222] are used to convert specific gravity data to density ( $\text{g}/\text{cm}^3$ ) values. The table of Douglas [3163] is used to convert reported temperatures to the IPTS-68 scale as necessary. The gas constant value used is  $8.31441 \text{ kPa cm}^3/\text{mol K}$ .

It is assumed that the old milliliter is related to the cubic centimeter by

$$0.999972 \text{ ml} = 1.0 \text{ cm}^3$$

However, it is usually not certain whether the data are reported in terms of the old milliliter or of the new milliliter which is equivalent to the cubic centimeter. Hence it is necessary to operate under arbitrary rules which hopefully maximize the probability of being correct in any given instance.

If the units are not specifically defined in a document, specific gravity values are assumed to be in  $\text{g}/\text{ml}(\text{old})$  and the 1.000028 factor is applied by the CON program. If the data are described as "density" data, the values are assumed to be  $\text{g}/\text{cm}^3$ . However, when checking the transcriber's work, the evaluator can change the unit code on specific gravity data from  $\text{g}/\text{ml}(\text{old})$  to  $\text{g}/\text{cm}^3$  if he thinks it probable that the authors used the new milliliter. Unfortunately, it is usually impossible to determine whether or not the 1.000028 correction factor should be applied.

The temperature scale used is also a matter of conjecture in most cases. Very few documents identify the temperature scale used. In such cases, the IPTS-68 scale is assumed for papers published in 1972 and later; the three-year lag is based on the assumptions that the data appeared in print one or two years after its measurement, and that the laboratory reporting the data probably would not have converted to the new scale until a year or two after the 1968 scale was announced. For papers published in 1971 and earlier years, all the data are assumed to be on the 1948 temperature scale; i.e., the only two temperature scales recognized by the CON programs are the 1948 and 1968 scales. Again, the evaluator can change the temperature scale code entered by the transcriber if he thinks the blanket rule might not apply.

#### 4. Evaluation Procedures

##### 4.1. Compound Constants

Of the compound constants subjected to a selection process, only the triple point and melting point are independent of the temperature-dependent correlations developed for the vapor pressure and the liquid density. Whenever a temperature-dependent correlation can be established for the vapor pressure, the recommended normal boiling point, critical temperature, critical pressure and acentric factor values reported come from that correlation. Similarly, the critical volume value comes from the liquid density correlation, as would the 20 and 25 °C densities if needed by the user. The critical compressibility factor  $Z_c$  is calculated from the  $T_c$  and  $P_c$  values from the vapor pressure correlation and the  $V_c$  value from the liquid density correlation using an R value of 8.31441 kPa cm<sup>3</sup>/mol K.

Before the vapor pressure and liquid density data are processed, tentative values of the compound constants (except for the dipole moment and the radius of gyration) are selected from the available literature values using program CONCON. Data from the major relevant compilations [1051, 1146, 3270, 3375, 41765] are transcribed directly onto the CONCON input forms. The 20 and 25 °C density values and the critical density values from all the 2956 ketone documents are transcribed first as density data input (program DENCON) and then copied onto the CONCON input forms. Similarly, the normal boiling point and critical temperature and pressure values are first transcribed as vapor pressure data (program VAPCON) and then copied for CONCON. Of all the compound constants, only the triple and melting points are transcribed in a separate pass through the 2956 documents. Actually, the person looking for triple and melting point values also transcribes critical property values; this dual coverage for the critical properties is made to decrease the probability of missing any critical point data.

Once the CONCON input file is complete, the program is used to convert all the input values to the processing units and list the literature values for each property (20° liquid density, 25° liquid density, triple point, melting point, normal boiling point, critical temperature, critical pressure, critical density and critical volume) in the order of ascending MRL numbers. All the temperatures are corrected to the IPTS-68 temperature scale except for those related to the 20° and 25 °C density values; those are allowed to remain as 293.15 and 298.15 K.

In the column of numbers for each property for each compound, the evaluator marks a tentative selected value. In the selection of those tentative values, the evaluator relies heavily upon the values reported by the major compilations of selected values, namely those of Ambrose [41765], the Thermodynamics Research Center at Texas A&M [3270], Kudchadker et al. [1051], and Kobe et al. [3375]. A value other than the one reported by the most recent of the above four compilations will be selected only if justified by the publication of high-quality values since the publication date of the compilation.

There is seldom any reason to change the initially selected values for the triple point and melting point, and the values marked on the CONCON print-out are usually the final values.

The tentative values selected for the 20° and 25 °C liquid densities and the normal boiling point are used as guide-lines in fixing the temperature correlations for the density and vapor pressure but, once those correlations are established, the selected values almost invariably have to be changed to conform to the correlations.

Whether or not the initially selected critical point values are changed depends upon the relative strengths of those initially selected critical point values and the high-temperature vapor pressure or liquid density data with which the selected critical values have to be matched. When the initially selected critical point values are believed to be firmer than the high-temperature data, the correlation is forced to pass through that selected critical point and any high-temperature data points which disagree too badly are discarded. If there is a set of high-temperature vapor pressure or liquid density data which is of high-quality, but which has no associated critical point values and does not line up with the initially selected critical values, it is sometimes necessary to adjust the critical values to conform with the other data. If the initially selected critical values are of reasonably good quality, the adjustment necessary to achieve conformity is usually within the experimental error associated with the reported values. In any case, the compound constant values reported for the vapor pressure and liquid density are always those calculated from the temperature correlations for those two properties.

The requirement that the density and vapor pressure compound constants conform to the temperature correlations may or may not make the final values better than those in earlier compilations. If high-quality data sets are available in regions of the compound constants, the correlation values will be firm and reliable. If the temperature-dependent points being fitted have little to recommend them other than their existence, the calculated compound constants can be less accurate than values obtained in other ways. For example, if one assembled all of the reported normal boiling point (or 20° and 25 °C density) values for a group of similar compounds and then forced the selected values for the individual compounds to agree with assumed correlations with respect to carbon number, branching, etc., it is highly probable that the values thus obtained for a given compound would not fall on the correlation curve for the available temperature-dependent points in the region. Which is more accurate depends upon the relative accuracies of the two conflicting correlations. That can only be decided by an analysis of each case, and even then the final decision may have to be arbitrary. In this report, the main objective is to provide the best available temperature correlation equations for use on a computer, and it is necessary to report compound constants which are compatible with those correlations. However, when it is essential for the user to have the best possible value of a compound constant, the firmness of the temperature-correlation should be examined (number and sources of competing data sets, number of points fitted, root-mean-square-deviation, etc.) and, if found doubtful, the user should consider values from other sources, particularly those in the TRL tables [3270].

## 4.2. Vapor Pressure

### 4.2.1. Unit Conversion Step

All of the vapor pressure data which can be found for the compound class being processed in the relevant documents (2956 for the ketones) are transcribed on input forms for program VAPCON (the unit conversion program for vapor pressure data), sorted by compound, and keyed into a computer disk file denoted as ORIGP. Program VAPCON is then run with ORIGP as the input file. The VAPCON output goes to the CONVP (converted) disk file. Besides correcting the temperatures to the IPTS-68 scale and converting the pressure units to kilopascals as necessary, VAPCON fits the equation

$$\ln P' = A - \frac{B}{T} \quad (1)$$

to two selected data points ("anchor" points selected by the evaluator for each compound) and stores the residual (deviation from the equation) for each literature data point in the CONVP file. Those residuals are scanned to identify points with extraordinarily large residuals. If a large residual is due to a transcription or keying error, the ORIGP file is corrected; if not, the wild point is deleted from the ORIGP file. After the ORIGP file has been cleared of all erroneous and obviously inconsistent data points, program VAPCON is run again to provide a "clean" CONVP file for use as input to the plotting program GENPLT.

#### 4.2.2. Plotting Step

Program GENPLT plots the literature data points for each compound in the form of the VAPCON residuals versus temperature. The ordinate scale for each compound plot is automatically determined by the minimum and maximum residual values for the compound--the objective is to spread the data points as much as possible on the eight-inch high plots. A different plotting symbol is used for each literature document providing data, and those symbols are related to the documents' MRL numbers in a tabulation at the end of each compound plot. Up to 128 different symbols are available, but in practice an effort is always made to screen the data for commonly-used compounds (such as acetone) in order to reduce the number of literature sources listed in the ORIGP file to a number less than 100 before running VAPCON.

The evaluator's objective at this point is to establish the "track" where he believes the vapor pressure-temperature curve for each compound should lie on the residual plots. The tentative selected normal boiling and critical point values are important guides. In addition, each document providing data for a compound is inspected to determine the probable quality of each set of data.

For heavily-measured compounds, the tracks of the final correlations on the residual plots will be covered by more or less solid bands of data points, particularly near the normal boiling points. In order to expand those bands and obtain a better resolution of the data points near the desired tracks, the evaluator deletes from the input CONVP file all the outlying points which obviously are not going to be included in the final correlations and then runs GENPLT again.

For those compounds with sparse data, the first GENPLT plot is all that is needed. For a compound with a fairly large number of data points, the removal of the outlying points may permit the second GENPLT plot to expand sufficiently to distinguish between all the data sets. For heavily-measured compounds like acetone, three or four successive plots may be necessary. In addition to removal of the outlying points, the evaluator may find it necessary to restrict the temperature range for the next plot to that for the most heavily populated region. This may be necessary because eq (1) is a straight line cutting across the bow of the data points on a  $\ln P$  versus  $1/T$  plot, and it usually provides residuals which plot in a downwardly concave curve with negative values at both ends and positive values in the middle. By restricting the maximum and minimum temperature and residual limits in the compound's data set in the CONVP file, only the points in the heavily populated region can be plotted and made to expand to fill the entire eight-inch plot.

The GENPLT plots are, of course, just a mechanical aid for the basic evaluation process--the considered deletion of some points while retaining others. Often, the decision to delete or retain a point is made easy by that point's position relative to the bulk of the equally reliable points on a properly expanded residual versus temperature plot. After the easy decisions have been made, the final definition of the correlation track must be based on the evaluator's appraisal of the relative qualities of the remaining competing data points. The source of the data can be a deciding factor; one expects data from sources such as the U. S. National Bureau of Standards, the National Physical Laboratory of England, etc. to be good. One cannot place much reliance on the stated experimental errors in most papers but, nevertheless, the evaluator can usually draw some fairly firm conclusions about the quality of the data from the manner in which the data are presented. Also, when dealing with a large number of compounds, the evaluator soon identifies those workers whose data usually fall in or close to the tracks defined for the compounds. He also soon recognizes those workers whose data usually fall away from the final track when highly reliable data sets are available for a compound.

In any case, based on the residual plots and his judgment as to the relative merits of the various data sets, the evaluator establishes the tracks on the residual plots of what he believes the best available property temperature correlations to be. Data points which deviate from those tracks are deleted. It is not uncommon for part of an extensive literature data set to be retained while the rest is deleted; the errors involved in a measurement can change with temperature and it is not unusual for the data points for an extensive data set to begin to bend away from those of other reliable data sets.

In some cases, the track will run between two data points or two sets of data points, neither one of which falls on the selected track. Rather than delete both and leave the correlation unsupported in that region, the evaluator may retain both if he believes the least squares fit will be closer to the truth with those points in the data base. In other words, the objective in the deletion process is not to achieve the lowest possible root-mean-squared-deviation value; the objective is to establish a string of data points which will give a correlation equation which represents the true property-temperature relation as well as can be inferred from the available experimental evidence.

While working with the residual plots, the tendency is to retain doubtful points in the temperature gaps between reliable sets of data. It is not possible to tell from the plots whether or not those points will provide useful support for the correlation equation or--because they fall a little off the track--may actually accentuate any tendency an equation might have to weave in a region where the data points are sparse.

#### 4.2.3. Correlation Step

When the evaluator has gone as far as allowed by the residual plots in the definition of the final temperature correlations, the CONVP disk file (now reduced in size) is used as input to program CARDSORT which produces the SORTP file as output. CARDSORT merges the literature data sets for each compound and puts the data points in each of the resulting sets in the order of ascending temperature. The SORTP file then serves as the input for the vapor pressure fitting program PFIT.

The vapor pressure correlation equations contained in PFIT are shown in Table 2. The Riedel [838], Frost-Kalkwarf [2372], Riedel-Plank-Miller-2 [4529], and Wagner [40337] equations each contain only four constants while the Vapres-2 equation has five. Only the Wagner equation is a reduced equation.

Even a five-constant equation has a tendency to weave (irregular first and second temperature derivatives) when fitted to less than perfect data over a wide temperature range. Also, users of correlations often object to equations with a large number of constants. Hence, the vapor pressure equations used have been restricted to the relatively simple forms shown in Table 2.

On the other hand, even a five-constant equation will often not fit good smooth data within experimental error all the way from the melting point to the critical point. These conflicting considerations forced the use of the following four temperature ranges for the computer storage of vapor pressure data.

| <u>Range</u> | <u>Temperature range, K</u> |
|--------------|-----------------------------|
| 1            | $T_m$ to $T_c$              |
| 2            | $T_m$ to ( $T_b$ + 20)      |
| 3            | $T_m$ to $T_d$              |
| 4            | ( $T_b$ - 20) to $T_c$      |

The  $T_m$ ,  $T_b$  and  $T_c$  are the melting, normal boiling and critical temperatures, and  $T_d$  is defined by  $T_d = 0.85 T_c$ . When  $T_c$  is not available, a  $T_d$  value is calculated from  $T_d = 1.45 T_b$ .

Table 2. Vapor pressure correlation equations used

|                       |  |
|-----------------------|--|
| Riedel                | $\ln_e P' = A + B \ln_e T + \frac{C}{T} + DT^6$  |
| Frost-Kalkwarf        | $\ln_e P' = A + B \ln_e T + \frac{C}{T} + \frac{DP'}{T^2}$   |
| Riedel-Plank-Miller-2 | $\ln_e P' = A + \frac{B}{T} + CT + DT^2$   |
| Vapres-2              | $\ln_e P' = A + \frac{B}{T} + CT + DT^2 + E \ln_e T$   |
| Wagner                | $\ln_e P'_r = A \frac{1-T_r}{T_r} + B \frac{(1-T_r)^{1.5}}{T_r} + C \frac{(1-T_r)^3}{T_r} + D \frac{(1-T_r)^6}{T_r}$ |

The order of priority for the use of the fits insofar as the accuracy of the fits is concerned is 2, 4, 3 and 1. The Range 1 fit is included for the user who is not particularly concerned about the best possible accuracy and does not want to worry about changing correlations in order to cover a wide temperature range.

In general, the equation form used to correlate the data for a given compound in a given temperature range is the one which best represents the selected data points. In the first PFIT run, the evaluator requests fits from all those equations which he believes might work well for each compound-range combination. From those results, the evaluator first selects the equation which works best for each compound-range combination, and then proceeds with any further data point deletions needed to achieve the final correlations.

The PFIT printout has several characteristics which aid in the selection of additional points to be deleted and in judging the performance of the equation used. First, the percent deviation of each point from the equation value is given. Second, the deviation of each point is displayed in terms of a positive or negative multiple of the root-mean-squared-deviation for the entire fit. Third, the normal boiling and critical point values calculated from the equation are compared to the tentative selected values. Fourth, the root-mean-squared-deviation for the fit is given and the maximum deviation point is identified. Fifth, the number of positive deviations and the number of negative deviations from the equation are given. Both of the first two items are necessary because of the very large change in the magnitude of the vapor pressure. At low temperatures, all the RMSD multiples are close to zero and the percent deviation values must be used. At high temperatures, the RMSD multiple display is more useful. That display, plus the numbers in the fifth item make it possible to tell at a glance whether the equation is splitting the data points or crossing back and forth across them.

After the first round of point deletions based on the first fits, PFIT is run the second time with a greatly reduced number of equation selections. Multiple equation selections may still be used for some compound-range combinations if the initial fits were competitive and it is felt that the new point deletions might affect the final choice. Based on the second PFIT run, the evaluator makes his final equation selections and may still decide to trim away a data point here and there. He may also decide to insert again some points deleted in the previous round. Usually all the correlations are fixed after the second PFIT run. PFIT is then run the third time to provide the final set of correlation constants and store them in a form which will facilitate the storage in the data bank.

In each of its runs, the "weave" check option in PFIT is used. That option requests the calculation and tabulation (as a function of temperature) of the first and second derivatives of  $P'$  and  $\ln P'$  from each equation fit based on fewer than 30 data points. The derivative tabulations permit the evaluator to identify those fits which weave or take on odd slope values when the experimental data points are sparse and scattered. The five-constant Vapres-2 equation exhibits such behavior much more often than the four-constant equations.

On the final PFIT run, the boiling point and storage options in PFIT are also used. The storage option creates a disk file of the correlation constants. The boiling point option causes the calculation of the normal boiling point from each correlation equation. The evaluator then selects the value from either the range 2 or range 4 fits as the final selected value to replace the tentative value marked on the CONCON printout. The choice between the two ranges is based on (a) how closely each correlation fits the data points in the region of the boiling points, (b) which value agrees best with the tentative selected value, and (c) the relative firmness of the tentative selected value and the experimental data points being fitted. For well-studied compounds, the difference between the tentative and final selected values will usually be less than a few hundredths of a degree. For compounds where the normal boiling point is still a matter of conjecture, the difference can be as high as two or three degrees.

As explained in section 4.1, any necessary adjustments of the tentative  $T_c$  and  $P_c$  values will have been made before the final PFIT run, and there is no need to calculate new values consistent with the correlation equations. In short, the correlations are made to conform with the selected critical point values rather than vice versa.

When  $T_c$  and  $P_c$  values are available, the reduced Wagner equation is almost invariably used for those two ranges (1 and 4) which include the critical point; that is done to force an exact fit of the selected critical point values. Because it must go through the critical point, the Wagner equation is not as free to fit the other data points and, in relatively rare instances, the Riedel equation is used for ranges 1 and 4 if it reproduces the critical point closely enough and at the same time gives a better fit of the rest of the data than does the Wagner equation. The Riedel-Plank-Miller-2 equation is usually chosen for Ranges 2 and 3 when the data points are relatively sparse and scattered; that equation very seldom exhibits unreasonable temperature derivatives. If there are a lot of points in Ranges 2 and 3, the Riedel and Vapres-2 equations may be competitive.

The Vapres-2 equation is often useful when two good but separated data sets are available. For example, there may be a data set at very low temperature (close to the melting point), another set in the normal boiling point region, and a large gap between them with only miscellaneous scattered data points. It is usually difficult to tie two such data sets together without large deviations at both ends of the gap. Because of its fifth constant, the Vapres-2 equation is often more flexible in such situations.

The Frost-Kalkwarf equation is seldom used. In early work on a large number of hydrocarbons, it seldom showed any advantage over the other equations and its use gradually declined because of the inconvenience due to the presence of  $P'$  on both sides of the equation.

### 4.3. Liquid Density

#### 4.3.1. Unit Conversion Step

The liquid density data processing procedures are similar to those described in section 4.2 for the vapor pressure data. All the literature data which can be found are keyed into the ORIGD disk file. Program DENCON corrects the temperatures to the IPTS-68 scale and the density or volume units to  $\text{g cm}^{-3}$  as necessary, and stores the converted literature data in the CONVD file. DENCON also calculates and stores a residual value for each data point based on a quadratic fit of three "anchor" density points selected from the input literature data by the evaluator. Those three points include one near the bottom of the temperature range, one near the top, and one at about three-fourths of the distance from the bottom to the top anchor point; those three points are chosen to allow the simple quadratic equation to approximate the density versus temperature curve near the critical region without generating inordinately large residuals. The special problems encountered in the unit conversions for density data have been discussed in section 3.

*crud*

Erroneous and obviously inconsistent data points are identified and cleared from the ORIDG file as described in section 4.2.1 for the vapor pressure data. Then DENCON is run the second time to create a clean CONVD file for the plotting step.

#### 4.3.2. Plotting Step

Program GENPLT is used to plot the density data in exactly the same way as described for vapor pressure. On one hand, the density data are easier to plot because the data values cover such a small numerical range. On the other hand, the quadratic is not as good for fitting density data as is the equation used for vapor pressure and hence the residuals sometimes are more erratic, particularly when the data extend to the critical point. Nevertheless, it is usually necessary to plot the density data fewer times than the vapor pressure data.

The 20° and 25 °C density points serve as guidelines in exactly the same way as the normal boiling point is used for vapor pressure to establish the correlation "track" on the residual plots, and the reasons for adjusting or not adjusting the tentative selected critical point values are the same as described in section 4.2.2. Also, the same approach is used in making the point deletion decisions.

#### 4.3.3. Correlation Step

Once the evaluator has finished making deletions in the CONVD file based on the residual plots, program CARDSORT is used to merge the literature data sets for each compound and order those points with respect to temperature. The newly-ordered data are stored in the SORTD disk file.

The three density correlation equations used to fit the density data are shown in Table 3. Those three equations are contained in separate programs instead of being combined in one program as done for the vapor pressure. The low-temperature range Francis equation [4094] is in program FRANCIS1, and the high range Francis equation is in program FRANCIS2. The Rackett equation [4121, 4123] is applied by program RACKETT.

The temperature ranges used for the liquid density fits differ from those for the vapor pressure because of the difference in the shapes of the two property curves and the differences in the correlation equations. The low-range Francis equation can be fitted to the following ranges using program FRANCIS1.

| <u>Range</u> | <u>Temperature Range, K</u>  |
|--------------|------------------------------|
| 1            | $T_m$ to $(T_c - 10)$        |
| 2            | $T_m$ to $(T_b + 20)$        |
| 3            | $T_m$ to $(T_c - 30)$        |
| 4            | $(T_b - 20)$ to $(T_c - 10)$ |

Francis [4094] recommended that his low-range equation be restricted to temperatures below  $(T_c - 30)$  and the range 3 fit observes that limit. However, it is sometimes possible to fit up to  $(T_c - 10)$  without serious loss of accuracy and the extended range is sometimes needed to overlap the fit obtained with his high range equation.

Table 3. Liquid density correlation equations used

---

|                                 |   |
|---------------------------------|---|
| Francis, < (T <sub>c</sub> -10) | $d = A - BT - \frac{C}{E-T}$  |
| Francis, > (T <sub>c</sub> -50) | $d = [A(T_c - T)]^{1/B} + d_c$  |
| Rackett                         | $\frac{V^L}{FW} = \frac{1}{d} = \frac{8.31441 T_c}{(FW)P_c} Z_{RA}^{[1+(1-T_r)^{2/7}]}$ |

---

The high-range Francis equation (program FRANCIS2) is restricted to the  $(T_c - 50)$  to  $T_c$  range. Francis [4094] stated that the equation performed fairly well down to 50 to 100 degrees below the critical point. However, the region near the critical is difficult to fit without large percentage errors. That difficulty is caused by a combination of factors. First, the density curve near the critical is very steep and a small temperature error can cause a large deviation for a data point. Second, a short distance from the critical point the slope begins a rapid change to a small value. Third, the high-range Francis equation must pass through the critical point and quite often the selected  $d_c$  value will not be entirely consistent with the data points near the critical temperature. Hence, it is better to limit the high-range equation to a 50 K increment and stretch the low-range equation fits upward for the FRANCIS1 fits for ranges 1 and 4.

The Rackett equation is never competitive with the low-range Francis equation over the ranges 1, 2 and 3 used in program FRANCIS1. Hence, its use is restricted to the same  $(T_c - 50)$  to  $T_c$  range used by program FRANCIS2, but it is also seldom competitive with the high-range Francis equation.

The low-range Francis equation is a very reliable correlation equation and will always fit well within experimental accuracy any good set of data in range 2. The range 3 fit may sometimes fall a little out of the experimental error band because of the wide temperature range covered. The range 4 fit would be as good as the range 2 fit if the range were cut back to  $T_c - 20$  or  $T_c - 30$ , but the small loss of accuracy sometimes caused by the extended temperature range is not an unreasonable price to pay. Also, the low-range Francis equation is remarkably free of slope problems when fitting sparse, scattered data points. In short, the low-range Francis equation is a very satisfactory correlation equation as long as one does not get too close to the critical points.

The low-range Francis equation fits are always used for the ranges 1, 2 and 3 as defined above for program FRANCIS1. When the data do not extend all the way to the critical, the FRANCIS1 range 4 fit is also used. If the data do extend to the critical, then a choice must be made between the FRANCIS1 range 4 fit and the  $(T_c - 50)$  to  $T_c$  fit from FRANCIS2 (and possibly RACKETT).

The choice is easy if the FRANCIS2 (or RACKETT) fit is good. Then the FRANCIS2 or RACKETT fit over the  $(T_c - 50)$  to  $T_c$  range is chosen for the range 4 correlation and overlapping fits are available from  $T_m$  to  $T_c$ . Sometimes the percentage errors in the FRANCIS2 fit are so large (for reasons described above) that the evaluator decides that coverage of the  $(T_c - 10)$  to  $T_c$  range is not feasible. He then chooses the FRANCIS1 range 4 fit for the final range 4 correlation.

The FRANCIS1, FRANCIS2 and RACKETT printouts provide the evaluator with the same information as the PFIT printout to aid in the selection of points to be deleted and to aid in judging the quality of the equation fits. However, the "weave" option is not necessary for the density programs because the Francis equations are not as subject to slope problems as the vapor pressure equations. Also, the final density correlation equations are not asked to calculate values of the 20 and 25 °C densities. Only the option requesting disk storage of the correlation constants is used on the final fitting runs.

#### 4.4. Second Virial Coefficient

The second virial coefficient data are not subjected to the extensive evaluation process applied to vapor pressure and liquid density data. The objective is just to select that predictive correlation equation which best represents the better literature data sets for each compound.

Six predictive equations are always tested: Kreglewski [6771], Pitzer and curl [6288], O'Connell-Prausnitz [897], Tsonopoulos [11414], Nothnagel-Abrams-Prausnitz [9819], Hayden-O'Connell [8531]. No attempt is made to adjust the correlation constants; i.e., no least-squares data fitting is done.

The data processing for the second virial coefficient data starts like that for the vapor pressure and liquid density. All the literature data are first transcribed from the relevant literature documents onto input forms for program BCON. (Some data sets beyond those appearing in the Dymond and Smith [41648] compilation are usually found but they very seldom are of any significance. The Dymond and Smith book has been found to be an exhaustive compilation of existing good literature data.) The transcribed data are keyed into disk file ORIGB which serves as input to program BCON. BCON stores the converted B values in disk file CONVB.

Second virial data are reported in the literature for each of the following equations:

$$PV = A(1 + B/V + C/V^2 + \dots) \quad (2a)$$

$$PV = A' + B'/V + C'/V^2 + \dots \quad (2b)$$

$$PV = A*(1 + B^*P + C^*P^2 + \dots) \quad (2c)$$

$$PV = A'' + B''P + C''P^2 + \dots \quad (2d)$$

The relations between the various second coefficients is

$$B = B'/RT = RTB^* = B'' \quad (3)$$

BCON converts all the literature second coefficient values as necessary to B values (eq (2a)) in terms of  $\text{cm}^3 \text{ mol}^{-1}$ . It also converts the data point temperatures to the IPTS-68 scale as necessary.

The BCON input file (ORIGP) must contain the correlation constants for each correlation to be tested. Those constants are taken from the literature documents for the individual correlations. All correlations for which constants can be found are always tested.

Using the CONVB disk file as input, program GENPLT produces a residual plot for each equation tested for each compound for which B values could be found in the literature. Data were found for the following ketones.

| ID     | compound              |
|--------|-----------------------|
| KE0300 | acetone (2-propanone) |
| KE0400 | 2-butanone            |
| KE0500 | 2-pentanone           |
| KE0501 | 3-pentanone           |
| KE0505 | 2-methyl-2-butanone   |
| KE0601 | 3-hexanone            |

The significance of the ID number will be explained later; here it is just used as a convenient tag for the compounds in Table 4 where the test results for the various correlations are summarized.

The BCON printout gives the root-mean-squared deviation for each set of literature data for each correlation tested. Those values are listed in Table 4. BCON also gives the rmsd value for the combined data sets for each compound but that number is not very useful because the individual data sets vary in quality and the selection of the best correlation must be based on those few data sets which are felt to be of the highest quality.

Table 4. Correlation test results for second virial coefficient data

| ID     | Reference number | Root-mean-squared-deviation for data set |        |           |             |           |        |
|--------|------------------|--|--------|-----------|-------------|-----------|--------|
|        |                  | Kreglewski                               | Pitzer | O'Connell | Tsonopoulos | Nothnagel | Hayden |
| KE0300 | 1257             | 176                                      | 480    | 190       | 168         | 199       | 129*   |
| KE0300 | 1803             | 46                                       | 247    | 45        | 24*         | 96        | 38     |
| KE0300 | 1950             | 147*                                     | 972    | 548       | 265         | 148       | 277    |
| KE0300 | 2422             | 84                                       | 261    | 117       | 96          | 67*       | 115    |
| KE0300 | 2678             | 35                                       | 294    | 74        | 24*         | 69        | 51     |
| KE0300 | 5214             | 80                                       | 460    | 137       | 107         | 95        | 67*    |
| KE0300 | 5283             | 72                                       | 307    | 48        | 45*         | 77        | 72     |
| KE0300 | 5948             | 15*                                      | 378    | 115       | 50          | 32        | 52     |
| KE0300 | 8330             | 71                                       | 676    | 282       | 62          | 59*       | 70     |
| KE0300 | 8577             | 19*                                      | 524    | 194       | 80          | 32        | 71     |
| KE0300 | 9027             | 145                                      | 493    | 260       | 181         | 124*      | 188    |
| KE0300 | 10972            | 47                                       | 360    | 42        | 12*         | 49        | 46     |
| KE0300 | 20469            | 46                                       | 247    | 45        | 24*         | 96        | 38     |
| KE0400 | 10901            | 28*                                      | 327    | 462       | 83          | 59        | 28     |
| KE0400 | 21584            | 96                                       | 332    | 452       | 64*         | 121       | 89     |
| KE0500 | 10901            | 37*                                      | 471    | 701       | 164         | 607       | 369    |
| KE0501 | 4033             | 180                                      | 430    |           | 21*         | 87        |        |
| KE0501 | 21584            | 124                                      | 219    |           | 92*         | 103       |        |
| KE0505 | 4033             | 185                                      | 316    |           | 140*        |           |        |
| KE0601 | 4033             |  | 359    |           | 29*         |           |        |

The correlation equation which gave the lowest rmsd value for each set of data is indicated by an asterisk on that lowest value in Table 4. The Tsonopoulos equation was the best performer, giving the lowest rmsd for 10 of the 20 literature data sets. The Kreglewski correlation was the second best performer with the lowest rmsd for 5 sets of data. However, the use of the Kreglewski correlation is restricted to pure compound calculations because there are no mixing rules for mixture calculations, hence it is of less intrinsic interest than the other correlations.

Comparison of the rmsd for all the literature data sets can be misleading because the best correlation should not give the lowest rmsd for a bad set of data. Of the 13 literature data sets for acetone (KE0300), Dymond and Smith [41648] favor the Hajjar et al. [1803], Bottomley et al. [2678] and Knoebel et al. [5948] sets, with preference given to the first two sets above 360 K. The Tsonopoulos correlation gives the lowest rmsd for the first two while the Nothnagel et al. equation fits the third set best, hence the Tsonopoulos equation was chosen for acetone.

For 2-butanone (KE0400), the Hayden-O'Connell correlation's rmsd was lower than that of the Tsonopoulos equation for the Nickerson et al. [10901], and also lower for the combined Nickerson et al. and the Chang et al. [21584] set. Hence, the Hayden-O'Connell correlation was chosen for 2-butanone.

The Tsonopoulos correlation was chosen for all of the rest of the compounds in Table 4. The Kreglewski correlation represented the 2-pentanone data much better but, because of the lack of mixture mixing rules, that equation is never chosen for storage in the data bank.

## 5. Selected Values

The objective was to select the best values from all the available literature data for each relevant compound-property combination. For heavily-measured compounds, the selected values should be quite accurate. For sparsely-measured compounds, the selected values often have little to recommend them other than the fact that they appear to be the best of the limited information available.

Table 5 lists those compounds for which enough information was found to merit inclusion in this report. Table 5 also gives the identification numbers which are used to identify the compounds in succeeding tables. The first two characters of the "number" are always alphabetical and represent the compound class (KE for ketones, OH for alcohols, etc.). The second two characters are related to the carbon number as shown in Table 6. It was possible to use the carbon number as the second two characters only through 8. For carbon numbers 9 and 10, more than 100 numbers has been needed for some compound classes. The ranges for those two carbon numbers were made overly large in order to get back to a more obvious relationship between carbon number and the identification number starting with carbon number 11.

Chemical nomenclature is a serious problem when retrieving information from a computer data bank. To alleviate that problem, up to four different compound names can be stored with each compound record. Table 5 lists all the names used for each compound.

Table 5. Compound identification numbers

|        |  |
|--------|--|
| KE0300 | ACETONE                                    |
| KE0300 | 2-PROPANONE                                |
| KE0305 | HEXADEUTEROACETONE                         |
| KE0305 | ACETONE-D(6)                               |
| KE0340 | 1-HYDROXY-2-PROPANONE                      |
| KE0340 | ACETYLCARBINOL                             |
| KE0360 | 1-CHLORO-2-PROPANONE                       |
| KE0360 | CHLOROACETONE                              |
| KE0361 | 1,1-DICHLORO-2-PROPANONE                   |
| KE0361 | 1,1-DICHLOROACETONE                        |
| KE0362 | 1,3-DICHLORO-2-PROPANONE                   |
| KE0362 | 1,3-DICHLOROACETONE                        |
| KE0370 | 1-CHLORO-1,1,3,3,3-PENTAFLUORO-2-PROPANONE |
| KE0370 | PENTAFLUOROCHLOROACETONE                   |
| KE0370 | CHLOROPENTAFLUOROACETONE                   |
| KE0380 | 1,1,1,3,3,3-HEXAFLUORO-2-PROPANONE         |
| KE0380 | PERFLUOROACETONE                           |
| KE0380 | HEXAFLUOROACETONE                          |
| KE0400 | 2-BUTANONE                                 |
| KE0400 | METHYL ETHYL KETONE                        |
| KE0400 | ETHYL METHYL KETONE                        |
| KE0410 | 2,3-BUTANEDIONE                            |
| KE0410 | BIACETYL                                   |
| KE0410 | DIACETYL                                   |
| KE0420 | CYCLOBUTANONE                              |
| KE0430 | 1,3-CYCLOBUTANEDIONE                       |
| KE0430 | CYCLOBUTAN-1,3-DIONE                       |
| KE0440 | 3-BUTEN-2-ONE                              |
| KE0440 | METHYL VINYL KETONE                        |
| KE0440 | VINYL METHYL KETONE                        |
| KE0445 | 3-HYDROXY-2-BUTANONE                       |
| KE0445 | ACETOIN                                    |
| KE0445 | ACETYL METHYL CARBINOL                     |
| KE0446 | 4-HYDROXY-2-BUTANONE                       |
| KE0446 | 3-KETOBUTANOL                              |
| KE0450 | 1-BROMO-2-BUTANONE                         |
| KE0450 | BROMOMETHYL ETHYL KETONE                   |
| KE0451 | 3-BROMO-2-BUTANONE                         |
| KE0451 | METHYL 1-BROMOETHYL KETONE                 |
| KE0460 | 3-CHLORO-2-BUTANONE                        |
| KE0460 | 3-CHLOROBUTANONE-2                         |
| KE0500 | 2-PENTANONE                                |
| KE0500 | METHYL N-PROPYL KETONE                     |
| KE0500 | METHYL PROPYL KETONE                       |
| KE0501 | 3-PENTANONE                                |
| KE0501 | DIETHYL KETONE                             |
| KE0501 | PROPIONE                                   |
| KE0505 | 3-METHYL-2-BUTANONE                        |
| KE0505 | ISOPROPYL METHYL KETONE                    |

Table 5. Compound identification numbers--Continued

|        |                                |
|--------|--------------------------------|
| KE0505 | METHYL ISOPROPYL KETONE        |
| KE0510 | 2,4-PENTANEDIONE               |
| KE0510 | ACETYLACETONE                  |
| KE0510 | DIACETYLMETHANE                |
| KE0520 | CYCLOPENTANONE                 |
| KE0520 | ADIPIC KETONE                  |
| KE0520 | KETOPENTAMETHYLENE             |
| KE0530 | ACETYLCYCLOPROPANE             |
| KE0530 | METHYL CYCLOPROPYL KETONE      |
| KE0530 | CYCLOPROPYL METHYL KETONE      |
| KE0530 | 1-CYCLOPROPYL-1-ETHANONE       |
| KE0540 | 3-METHYL-3-BUTEN-2-ONE         |
| KE0540 | METHYL ISOPROPENYL KETONE      |
| KE0555 | 4-BROMO-2-PENTANONE            |
| KE0555 | 2-BROMOPROPYL METHYL KETONE    |
| KE0563 | 1-HYDROXY-3-METHYL-2-BUTANONE  |
| KE0563 | BETA-METHYL-ALPHA-KETOBUTANOL  |
| KE0565 | 3-HYDROXY-3-METHYL-2-BUTANONE  |
| KE0566 | 4-HYDROXY-3-METHYL-2-BUTANONE  |
| KE0568 | 1-HYDROXY-4-METHOXY-2-BUTANONE |
| KE0570 | 5-HYDROXY-3-PENTYN-2-ONE       |
| KE0570 | 1-HYDROXY-2-PENTYNE-4-ONE      |
| KE0600 | 2-HEXANONE                     |
| KE0600 | METHYL BUTYL KETONE            |
| KE0600 | BUTYL METHYL KETONE            |
| KE0601 | 3-HEXANONE                     |
| KE0601 | ETHYL PROPYL KETONE            |
| KE0604 | 4-METHYL-2-PENTANONE           |
| KE0604 | ISOBUTYL METHYL KETONE         |
| KE0604 | METHYL ISOBUTYL KETONE         |
| KE0604 | ISOPROPYL ACETONE              |
| KE0605 | 2-METHYL-3-PENTANONE           |
| KE0605 | ETHYL ISOPROPYL KETONE         |
| KE0607 | 3,3-DIMETHYL-2-BUTANONE        |
| KE0607 | TERT-BUTYL METHYL KETONE       |
| KE0607 | PINACOLONE                     |
| KE0607 | PINACOLIN                      |
| KE0610 | 2,5-HEXANEDIONE                |
| KE0610 | ACETONYL ACETONE               |
| KE0615 | 3-METHYL-2,4-PENTANEDIONE      |
| KE0615 | METHYLACETYLACETONE            |
| KE0620 | CYCLOHEXANONE                  |
| KE0620 | KETOHEXAMETHYLENE              |
| KE0620 | PIMELIC KETONE                 |
| KE0625 | 3-METHYLCYCLOPENTANONE         |
| KE0640 | 5-HEXEN-2-ONE                  |
| KE0640 | ALLYLACETONE                   |
| KE0645 | 4-METHYL-4-PENTEN-2-ONE        |
| KE0645 | ISOMESITYL OXIDE               |
| KE0650 | 4-METHYL-3-PENTEN-2-ONE        |
| KE0650 | ISOPROPYLIDENEACETONE          |

Table 5. Compound identification numbers--Continued

|        |                                       |
|--------|---------------------------------------|
| KE0650 | MESITYL OXIDE                         |
| KE0660 | 2,5-CYCLOHEXADIENE-1,4-DIONE          |
| KE0660 | 1,4-BENZOQUINONE                      |
| KE0660 | P-QUINONE                             |
| KE0660 | P-BENZOQUINONE                        |
| KE0670 | 4-HYDROXY-4-METHYL-2-PENTANONE        |
| KE0670 | DIACETONE ALCOHOL                     |
| KE0680 | 6-BROMO-2-HEXANONE                    |
| KE0680 | 6-BROMOHEXANE-2-ONE                   |
| KE0700 | 2-HEPTANONE                           |
| KE0700 | METHYL AMYL KETONE                    |
| KE0700 | METHYL PENTYL KETONE                  |
| KE0701 | 3-HEPTANONE                           |
| KE0701 | ETHYL BUTYL KETONE                    |
| KE0701 | BUTYL ETHYL KETONE                    |
| KE0702 | 4-HEPTANONE                           |
| KE0702 | DIPROPYL KETONE                       |
| KE0710 | 2-METHYL-3-HEXANONE                   |
| KE0710 | PROPYL ISOPROPYL KETONE               |
| KE0720 | 2,4-DIMETHYL-3-PENTANONE              |
| KE0720 | DIISOPROPYL KETONE                    |
| KE0720 | TETRAMETHYLACETONE                    |
| KE0720 | ISOBUTYRONE                           |
| KE0725 | 3,3-DIMETHYL-2,4-PENTANEDIONE         |
| KE0725 | DIMETHYL ACETYL ACETONE               |
| KE0730 | 3-ETHYL-2,4-PENTANEDIONE              |
| KE0730 | ETHYL ACETYL ACETONE                  |
| KE0735 | 2,4,6-HEPTANETRIONE                   |
| KE0735 | DIACETYL ACETONE                      |
| KE0740 | CYCLOHEPTANONE                        |
| KE0745 | 2-METHYL-1-CYCLOHEXANONE              |
| KE0745 | 2-METHYLCYCLOHEXANONE                 |
| KE0746 | 3-METHYL-1-CYCLOHEXANONE              |
| KE0746 | 3-METHYLCYCLOHEXANONE                 |
| KE0747 | 4-METHYL-1-CYCLOHEXANONE              |
| KE0747 | 4-METHYLCYCLOHEXANONE                 |
| KE0760 | 2-METHYL-2,5-CYCLOHEXADIENE-1,4-DIONE |
| KE0760 | 2-METHYL-1,4-BENZOQUINONE             |
| KE0760 | METHYL P-BENZOQUINONE                 |
| KE0800 | 2-OCTANONE                            |
| KE0800 | METHYL HEXYL KETONE                   |
| KE0801 | 3-OCTANONE                            |
| KE0801 | ETHYL AMYL KETONE                     |
| KE0802 | 4-OCTANONE                            |
| KE0802 | PROPYL BUTYL KETONE                   |
| KE0810 | 2-METHYL-3-HEPTANONE                  |
| KE0810 | ISOPROPYL BUTYL KETONE                |
| KE0830 | 2,5-DIMETHYL-3-HEXANONE               |
| KE0830 | ISOPROPYL ISOBUTYL KETONE             |
| KE0850 | 2,2,4-TRIMETHYL-3-PENTANONE           |
| KE0870 | ACETYL CYCLOHEXANE                    |

Table 5. Compound identification numbers--Continued

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|        |   |
|--------|---|
| KE0870 | 1-CYCLOHEXYL-1-ETHANONE                           |
| KE0870 | METHYL CYCLOHEXYL KETONE                          |
| KE0890 | CYCLOOCTANONE                                     |
| KE0910 | 2-PROPYL-1-CYCLOPENTANONE                         |
| KE0910 | ALPHA-PROPYLCYCLOPENTANONE                        |
| KE0930 | 3-ACETYL-5-HEXEN-2-ONE                            |
| KE0930 | ALLYL ACETYL ACETONE                              |
| KE0950 | ACETOPHENONE                                      |
| KE0950 | 1-PHENYLETHANONE                                  |
| KE0950 | METHYL PHENYL KETONE                              |
| KE0950 | ACETYLBENZENE                                     |
| KE0980 | 4-CHLOROACETOPHENONE                              |
| KE0980 | P-CHLOROACETOPHENONE                              |
| KE0980 | P-CHLOROPHENYL METHYL KETONE                      |
| KE1000 | 2-NONANONE  |
| KE1000 | METHYL HEPTYL KETONE                              |
| KE1001 | 3-NONANONE  |
| KE1001 | ETHYL N-HEXYL KETONE                              |
| KE1002 | 4-NONANONE  |
| KE1002 | PROPYL AMYL KETONE                                |
| KE1002 | AMYL PROPYL KETONE                                |
| KE1003 | 5-NONANONE  |
| KE1003 | DIBUTYL KETONE                                    |
| KE1003 | NONAN-5-ONE                                       |
| KE1020 | 2,6-DIMETHYL-4-HEPTANONE                          |
| KE1020 | DIISOBUTYL KETONE                                 |
| KE1040 | 2,2,4,4-TETRAMETHYL-3-PENTANONE                   |
| KE1040 | HEXAMETHYL ACETONE                                |
| KE1060 | 1-CYCLOHEXYL-1-PROPANONE                          |
| KE1100 | CYCLONONANONE                                     |
| KE1150 | 2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE                  |
| KE1150 | PHORONE   |
| KE1150 | DIISOPROPYLIDENEACETONE                           |
| KE1180 | 1-PHENYL-1-PROPANONE                              |
| KE1180 | PROPIOPHENONE                                     |
| KE1180 | ETHYL PHENYL KETONE                               |
| KE1180 | PHENYL ETHYL KETONE                               |
| KE1181 | 1-PHENYL-2-PROPANONE                              |
| KE1181 | BENZYL METHYL KETONE                              |
| KE1181 | PHENYL ACETONE                                    |
| KE1181 | ACETONYLBENZENE                                   |
| KE1200 | 4-METHYLACETOPHENONE                              |
| KE1200 | P-TOLYL METHYL KETONE                             |
| KE1200 | P-METHYLACETOPHENONE                              |
| KE1250 | 1-INDANONE  |
| KE1250 | ALPHA-HYDRINDONE                                  |
| KE1320 | 1-(2,2-DIMETHYLCYCLOPROPYL)-2-HYDROXY-1-PROPANONE |
| KE1320 | KETOL   |
| KE1350 | 3,5-DIBROMO-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE      |
| KE1350 | ALPHA,ALPHA'-DIBROMOPHORONE                       |
| KE1360 | 3,5-DICHLORO-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE     |

Table 5. Compound identification numbers--Continued

|        |   |
|--------|---|
| KE1360 | ALPHA, ALPHA'-DICHLOROPHORONE                             |
| KE1400 | 2-DECANONE  |
| KE1400 | METHYL OCTYL KETONE                                       |
| KE1401 | 3-DECANONE  |
| KE1401 | ETHYL N-HEPTYL KETONE                                     |
| KE1403 | 5-DECANONE  |
| KE1403 | BUTYL AMYL KETONE   |
| KE1500 | CYCLODECANONE   |
| KE1530 | 2-ISOPROPYL-5-METHYL-1-CYCLOHEXANONE                      |
| KE1530 | L-METHONE   |
| KE1530 | L-P-MENTHAN-3-ONE   |
| KE1530 | 1-METHYL-4-ISOPROPYL CYCLOHEXAN-3-ONE                     |
| KE1550 | 2,2,5,5-TETRAMETHYL-1-CYCLOHEXANONE                       |
| KE1550 | 1,1,4,4-TETRAMETHYL CYCLOHEXANONE-2                       |
| KE1580 | DECAHYDRO-2-NAPHTHALENONE                                 |
| KE1580 | TRANS-BETA-DECALONE                                       |
| KE1600 | 1,3,3-TRIMETHYL BICYCLO(2.2.1)HEPTAN-2-ONE                |
| KE1600 | FENCHONE  |
| KE1600 | 1,3,3-TRIMETHYL-2-NORCAMPHANONE                           |
| KE1620 | CAMPHOR   |
| KE1620 | 2-CAMPHANONE  |
| KE1620 | 1,7,7-TRIMETHYL BICYCLO(2.2.1)HEPTAN-2-ONE                |
| KE1640 | (1S)-1-ALPHA-ISOPROPYL-4-METHYL BICYCLO(3.1.0)HEXAN-3-ONE |
| KE1640 | ALPHA-THUJONE   |
| KE1640 | 3-THUJANONE   |
| KE1640 | TANACETONE  |
| KE1660 | 3-ISOPROPYL-6-METHYL-2-CYCLOHEXEN-1-ONE                   |
| KE1660 | CARVENONE   |
| KE1660 | 6-METHYL-3-(1-METHYLETHYL)-2-CYCLOHEXEN-1-ONE             |
| KE1680 | 5-ISOPROPYL-3-METHYL-2-CYCLOHEXEN-1-ONE                   |
| KE1680 | 1-METHYL-3-ISOPROPYL CYCLOHEXEN-6-ONE-5                   |
| KE1700 | 5-ISOPROPENYL-2-METHYL-2-CYCLOHEXEN-1-ONE                 |
| KE1700 | CARVONE   |
| KE1700 | 2-METHYL-5-(1-METHYLETHENYL)-2-CYCLOHEXEN-1-ONE           |
| KE1720 | 1-OXO-1,2,3,4-TETRAHYDRONAPHTHALENE                       |
| KE1720 | ALPHA-TETRALONE   |
| KE1720 | 3,4-DIHYDRO-1(2H)-NAPHTHALENONE                           |
| KE1750 | 1-PHENYL-1-BUTANONE                                       |
| KE1750 | PHENYL PROPYL KETONE                                      |
| KE1750 | PROPYL PHENYL KETONE                                      |
| KE1750 | BUTYROPHENONE   |
| KE1760 | 1-PHENYL-2-BUTANONE                                       |
| KE1760 | BENZYL ETHYL KETONE                                       |
| KE1762 | 4-PHENYL-2-BUTANONE                                       |
| KE1762 | BENZYL ACETONE  |
| KE1762 | METHYL-2-PHENYLETHYL KETONE                               |
| KE1800 | 3,5-DIMETHYLACETOPHENONE                                  |
| KE1820 | 3-ETHYLACETOPHENONE                                       |
| KE1820 | M-ETHYLACETOPHENONE                                       |
| KE1821 | 4-ETHYLACETOPHENONE                                       |
| KE1821 | P-ETHYLACETOPHENONE                                       |

Table 5. Compound identification numbers--Continued

|        |   |
|--------|---|
| KE1860 | 1-PHENYL-1,3-BUTANEDIONE                            |
| KE1860 | BENZOYLACETONE                                      |
| KE1900 | 1,3-DIACETYLBENZENE                                 |
| KE1900 | M-DIACETYLBENZENE                                   |
| KE1901 | 1,4-DIACETYLBENZENE                                 |
| KE1901 | P-DIACETYLBENZENE                                   |
| KE2000 | 5-BROMO-3-METHOXY-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE  |
| KE2000 | ALPHA-BROMO-ALPHA'-METHOXYPHORONE                   |
| KE2100 | 2-UNDECANONE  |
| KE2100 | 2-HENDECANONE                                       |
| KE2100 | METHYL N-NONYL KETONE                               |
| KE2104 | 6-UNDECANONE  |
| KE2104 | DI-N-AMYL KETONE                                    |
| KE2104 | UNDECAN-6-ONE                                       |
| KE2104 | DIAMYL KETONE                                       |
| KE2120 | CYCLOUNDECANONE                                     |
| KE2130 | 3-ACETOXY-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE          |
| KE2130 | ALPHA-ACETOXYPHORONE                                |
| KE2150 | 1-PHENYL-1-PENTANONE                                |
| KE2150 | N-BUTYL PHENYL KETONE                               |
| KE2150 | VALEROPHENONE                                       |
| KE2150 | PHENYL BUTYL KETONE                                 |
| KE2155 | 1-PHENYL-2-PENTANONE                                |
| KE2155 | BENZYL N-PROPYL KETONE                              |
| KE2170 | 2,2-DIMETHYL-1-INDANONE                             |
| KE2170 | BETA,BETA-DIMETHYL-ALPHA-HYDRINDON                  |
| KE2190 | 3-ACETOXY-5-BROMO-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE  |
| KE2190 | ALPHA-BROMO-ALPHA'-ACETOXYPHORONE                   |
| KE2225 | CYCLODODECANONE                                     |
| KE2235 | 5,5-DIETHYL-2,2-DIMETHYL-1-CYCLOHEXANONE            |
| KE2235 | 1,1-DIMETHYL-4,4-DIETHYLCYCLOHEXANONE-2             |
| KE2250 | 1-PHENYL-1-HEXANONE                                 |
| KE2250 | N-AMYL PHENYL KETONE                                |
| KE2250 | CAPROPHENONE  |
| KE2260 | 1-ACETYNAPHTHALENE                                  |
| KE2260 | 1-ACETONAPHTHONE                                    |
| KE2260 | METHYL 1-NAPHTHYL KETONE                            |
| KE2261 | 2-ACETYNAPHTHALENE                                  |
| KE2261 | 2-ACETONAPHTHONE                                    |
| KE2261 | METHYL 2-NAPHTHYL KETONE                            |
| KE2300 | 2-TRIDECANONE                                       |
| KE2300 | UNDECYL METHYL KETONE                               |
| KE2300 | METHYL UNDECYL KETONE                               |
| KE2300 | HENDECYL METHYL KETONE                              |
| KE2330 | 4-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-3-BUTEN-2-ONE |
| KE2330 | ALPHA-IONONE  |
| KE2331 | 4-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-3-BUTEN-2-ONE |
| KE2331 | BETA-IONONE   |
| KE2350 | 1-PHENYL-1-HEPTANONE                                |
| KE2350 | ENANTHOPHENONE                                      |
| KE2350 | HEXYL PHENYL KETONE                                 |

Table 5. Compound identification numbers--Continued

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|        |  |
|--------|--|
| KE2365 | BENZOPHENONE   |
| KE2365 | DIPHENYL KETONE  |
| KE2365 | BENZOYL BENZENE  |
| KE2365 | DIPHENYLMETHANONE  |
| KE2380 | 1-NAPHTHYL-1-PROPANONE                                       |
| KE2380 | 1-PROPIONAPHTHONE  |
| KE2380 | ETHYL 1-NAPHTHYL KETONE                                      |
| KE2430 | DIPHENYLETHANEDIONE  |
| KE2430 | BENZIL   |
| KE2430 | BIBENZOYL  |
| KE2430 | DIPHENYL-ALPHA,BETA-DIKETONE                                 |
| KE2445 | 1-(1-NAPHTHALENYL)-1-BUTANONE                                |
| KE2445 | N-PROPYL 1-NAPHTHYL KETONE                                   |
| KE2460 | 9,10-ANTHRACENEDIONE   |
| KE2460 | 9,10-ANTHRAQUINONE   |
| KE2460 | 9,10-DIOXOANTHRACENE   |
| KE2460 | ANTHRAQUINONE  |
| KE2473 | 1,4-DIHYDROXY-9,10-ANTHRACENEDIONE                           |
| KE2473 | QUINIZARIN   |
| KE2473 | 1,4-DIHYDROXYANTHRAQUINONE                                   |
| KE2474 | 1,5-DIHYDROXY-9,10-ANTHRACENEDIONE                           |
| KE2474 | 1,5-DIHYDROXYANTHRAQUINONE                                   |
| KE2477 | 1,8-DIHYDROXY-9,10-ANTHRACENEDIONE                           |
| KE2477 | 1,8-DIHYDROXYANTHRAQUINONE                                   |
| KE2506 | 8-PENTADECANONE  |
| KE2506 | DI-N-HEPTYL KETONE   |
| KE2506 | N-DIHEPTYL KETONE  |
| KE2506 | PENTADECANONE-8-ONE  |
| KE2540 | 1-PHENYL-1-NONANONE  |
| KE2540 | N-OCTYL PHENYL KETONE  |
| KE2545 | 1,3-DIPHENYL-2-PROPANONE                                     |
| KE2545 | DIBENZYL KETONE  |
| KE2565 | 1-(1-NAPHTHALENYL)-1-PENTANONE                               |
| KE2565 | N-BUTYL 1-NAPHTHYL KETONE                                    |
| KE2630 | 3-BENZOYLOXY-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE                |
| KE2630 | ALPHA-BENZOYLOXYPHORONE                                      |
| KE2645 | 1-(1-NAPHTHALENYL)-1-HEXANONE                                |
| KE2645 | N-PENTYL 1-NAPHTHYL KETONE                                   |
| KE2680 | 3-(4-BROMOBENZYLOXY)-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE        |
| KE2680 | ALPHA-P-BROMOBENZYLOXYPHORONE                                |
| KE2685 | 5-BROMO-3(4-BROMOBENZYLOXY)-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE |
| KE2685 | ALPHA-BROMO-ALPHA'-P-BROMOBENZYLOXYPHORONE                   |
| KE2688 | 3-BENZOYLOXY-5-BROMO-2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE        |
| KE2688 | ALPHA-BROMO-ALPHA'-BENZOYLOXYPHORONE                         |
| KE2707 | 9-HEPTADECANONE  |
| KE2707 | DIOCTYL KETONE   |
| KE2707 | N-HEPTADECANONE-9  |
| KE2745 | 1,5-DIPHENYL-1,4-PENTADIEN-3-ONE                             |
| KE2745 | DIBENZALACETONE  |
| KE2745 | DISTYRYL KETONE  |
| KE2755 | 1-(1-NAPHTHALENYL)-1-HEPTANONE                               |

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Table 5. Compound identification numbers--Continued

|        |                            |
|--------|----------------------------|
| KE2755 | N-HEXYL 1-NAPHTHYL KETONE  |
| KE2755 | HEPTANONAPHTHONE           |
| KE2775 | 7H-BENZ(DE)ANTHRACEN-7-ONE |
| KE2775 | BENZANTHRONE               |
| KE2835 | 1-PHENYL-1-DODECANONE      |
| KE2835 | N-UNDECYL PHENYL KETONE    |
| KE2835 | PHENYL UNDECYL KETONE      |
| KE2845 | 1-NAPHTHYL-1-OCTANONE      |
| KE2845 | N-HEPTYL 1-NAPHTHYL KETONE |
| KE2845 | OCTANONAPHTHONE            |
| KE2845 | CAPRYLONAPHTHONE           |
| KE3050 | 1-PHENYL-1-TETRADECANONE   |
| KE3050 | N-TRIDECYL PHENYL KETONE   |
| KE3050 | PHENYL TRIDECYL KETONE     |
| KE3310 | 12-TRICOSANONE             |
| KE3310 | DIUNDECYL KETONE           |
| KE3310 | LAURONE                    |
| KE3350 | 1-PHENYL-1-HEXADECANONE    |
| KE3350 | PENTADECYL PHENYL KETONE   |
| KE3350 | PALMITOPHENONE             |
| KE3712 | 14-HEPTACOSANONE           |
| KE3712 | DITRIDECYL KETONE          |
| KE3712 | MYRISTONE                  |
| KE4114 | 16-HENTRIACONTANONE        |
| KE4114 | DIPENTADECYL KETONE        |
| KE4114 | PALMITONE                  |
| KE4516 | 18-PENTATRIACONTANONE      |
| KE4516 | DIHEPTADECYL KETONE        |
| KE4516 | STEARONE                   |

Table 6. Relation between carbon number and  
the assigned compound identification number

| <u>Carbon<br/>number</u> | <u>Identification<br/>number</u> | <u>Carbon<br/>number</u> | <u>Identification<br/>number</u> | <u>Carbon<br/>number</u> | <u>Identification<br/>number</u> |
|--------------------------|----------------------------------|--------------------------|----------------------------------|--------------------------|----------------------------------|
| 1                        | 0100-0199                        | 11                       | 2100-2199                        | 21                       | 3100-3199                        |
| 2                        | 0200-0299                        | 12                       | 2200-2299                        | 22                       | 3200-3299                        |
| 3                        | 0300-0399                        | 13                       | 2300-2399                        | 23                       | 3300-3399                        |
| 4                        | 0400-0499                        | 14                       | 2400-2499                        | 24                       | 3400-3499                        |
| 5                        | 0500-0599                        | 15                       | 2500-2599                        | 25                       | 3500-3599                        |
| 6                        | 0600-0699                        | 16                       | 2600-2699                        | 26                       | 3600-3699                        |
| 7                        | 0700-0799                        | 17                       | 2700-2799                        | 27                       | 3700-3799                        |
| 8                        | 0800-0999                        | 18                       | 2800-2899                        | 28                       | 3800-3899                        |
| 9                        | 1000-1399                        | 19                       | 2900-2999                        | 29                       | 3900-3999                        |
| 10                       | 1400-2099                        | 20                       | 3000-3099                        | 30                       | 4000-4099                        |
|                          |                                  |                          |                                  | 31                       | 4100-4199                        |
|                          |                                  |                          |                                  | 32                       | 4200-4299                        |
|                          |                                  |                          |                                  | 33                       | 4300-4399                        |
|                          |                                  |                          |                                  | 34                       | 4400-4499                        |
|                          |                                  |                          |                                  | 35                       | 4500-4599                        |

A compound was included in Table 5 only if there was enough information to establish a temperature correlation for either vapor pressure or liquid density. To do that, there had to be at least two useable data points for at least one of those two properties. For example, liquid density values at 20° and 25 °C which gave a reasonable slope were sufficient to put a compound on the list even when no other data were available.

### 5.1. Compound Constants

The selected values of the compound constants are listed in Table 7. The 20 and 25 °C liquid density values are not included in the tabulation in order to make room for the dipole moment and radius of gyration, both of which are often needed for physical property correlations.

#### 5.1.1. Formula Weight

The atomic weights were taken from "Atomic Weights of the Elements 1975", Inorganic Chemistry Division Commission on Atomic Weights, International Union of Pure and Applied Chemistry, published in Pure and Applied Chemistry, 47, 75-95 (1976).

|           |           |
|-----------|-----------|
| Carbon    | 12.011    |
| Hydrogen  | 1.0079    |
| Deuterium | 2.016     |
| Bromine   | 79.904    |
| Chlorine  | 35.453    |
| Fluorine  | 18.998403 |
| Iodine    | 126.9045  |
| Nitrogen  | 14.0067   |
| Oxygen    | 15.9994   |

Table 7. Compound constant values

| ID     | FW      | MP, K   | NBP, K  | TC, K   | PC, MPa | VC, ml/mol | ZC    | $\omega$ | $\mu$ , Debye | R, $^{\circ}$ A |
|--------|---------|---------|---------|---------|---------|------------|-------|----------|---------------|-----------------|
| KE0300 | 58.080  | 178.476 | 329.207 | 508.100 | 4.700   | 208.921    | 0.232 | 0.3073   | 2.86          | 2.7404          |
| KE0305 | 64.128  |         |         |         |         |            |       |          |               |                 |
| KE0340 | 74.079  |         |         |         |         |            |       |          |               |                 |
| KE0360 | 92.525  |         | 391.656 |         |         |            |       |          | 2.38          |                 |
| KE0361 | 126.970 |         | 391.656 |         |         |            |       |          |               |                 |
| KE0362 | 126.970 | 316.139 | 445.185 |         |         |            |       |          |               |                 |
| KE0370 | 182.477 | 140.141 | 280.948 | 410.665 | 2.878   |            |       | 0.3449   |               | 4.0101          |
| KE0380 | 166.023 | 147.698 | 245.805 | 357.245 | 2.841   | 329.084    | 0.313 | 0.3649   |               | 3.8076          |
| KE0400 | 72.107  | 186.490 | 352.747 | 536.780 | 4.207   | 267.063    | 0.251 | 0.3220   | 2.78          | 3.1395          |
| KE0410 | 86.090  |         | 361.853 |         |         |            |       |          | 1.46          |                 |
| KE0420 | 70.091  | 222.179 | 371.990 |         |         |            |       |          | 2.61          | 2.7906          |
| KE0430 | 84.074  | 265.454 | 399.650 |         |         |            |       |          |               |                 |
| KE0440 | 70.091  |         | 354.703 |         |         |            |       |          | 3.00          |                 |
| KE0445 | 88.106  |         | 416.551 |         |         |            |       |          |               |                 |
| KE0446 | 88.106  |         | 455.150 |         |         |            |       |          |               |                 |
| KE0450 | 151.003 |         | 427.659 |         |         |            |       |          | 2.35          |                 |
| KE0451 | 151.003 |         | 409.159 |         |         |            |       |          |               |                 |
| KE0460 | 106.552 |         | 388.742 |         |         |            |       |          |               |                 |
| KE0500 | 86.133  | 196.320 | 375.408 | 561.080 | 3.694   | 301.164    | 0.238 | 0.3470   | 2.72          |                 |
| KE0501 | 86.133  | 234.203 | 375.109 | 561.460 | 3.729   | 336.457    | 0.268 | 0.3410   | 2.72          | 3.4817          |
| KE0505 | 86.133  | 181.178 | 367.482 | 553.400 | 3.850   | 309.831    | 0.259 | 0.3301   | 2.77          | 3.4148          |
| KE0510 | 100.117 | 249.964 | 411.855 |         |         |            |       |          | 2.81          |                 |
| KE0520 | 84.118  | 221.879 | 403.706 |         |         |            |       |          |               | 3.1662          |
| KE0530 | 84.118  | 204.883 | 384.870 |         |         |            |       |          | 2.87          |                 |
| KE0540 | 84.118  | 219.580 | 370.904 |         |         |            |       |          | 2.77          |                 |
| KE0555 | 165.030 |         |         |         |         |            |       |          |               |                 |
| KE0563 | 102.133 |         | 462.775 |         |         |            |       |          |               |                 |
| KE0565 | 102.133 |         | 416.404 |         |         |            |       |          |               |                 |
| KE0566 | 102.133 |         | 458.142 |         |         |            |       |          |               |                 |
| KE0568 | 118.132 |         |         |         |         |            |       |          |               |                 |
| KE0570 | 98.101  |         |         |         |         |            |       |          |               |                 |
| KE0600 | 100.160 | 217.381 | 400.733 | 587.000 | 3.323   |            |       | 0.3942   | 2.68          |                 |
| KE0601 | 100.160 | 217.531 | 396.656 | 582.820 | 3.320   |            |       | 0.3794   |               |                 |
| KE0604 | 100.160 | 189.181 | 388.856 | 571.000 | 3.270   |            |       | 0.3663   |               |                 |
| KE0605 | 100.160 |         | 388.032 |         |         |            |       |          |               |                 |
| KE0607 | 100.160 | 221.179 | 379.263 | 567.000 | 3.470   |            |       | 0.3229   | 2.81          |                 |
| KE0610 | 114.144 | 264.155 |         |         |         |            |       |          |               |                 |
| KE0615 | 114.144 |         |         |         |         |            |       |          |               |                 |
| KE0620 | 98.144  | 241.969 | 428.763 | 629.000 | 3.850   |            |       | 0.4524   | 3.08          |                 |
| KE0625 | 98.144  | 214.782 |         |         |         |            |       |          |               |                 |
| KE0640 | 98.144  |         | 402.144 |         |         |            |       |          |               |                 |
| KE0645 | 98.144  |         | 394.648 |         |         |            |       |          |               |                 |
| KE0650 | 98.144  |         | 402.959 |         |         |            |       |          | 3.24          |                 |
| KE0660 | 108.096 | 388.655 |         |         |         |            |       |          | .68           |                 |
| KE0670 | 116.160 | 226.177 | 441.076 |         |         |            |       |          | 3.24          |                 |
| KE0680 | 179.056 |         | 490.027 |         |         |            |       |          |               |                 |
| KE0700 | 114.187 | 238.171 | 424.206 | 611.500 | 3.436   |            |       | 0.4857   | 2.61          |                 |

Table 7. Compound constant values--Continued

|        |         |         |         |         |       |
|--------|---------|---------|---------|---------|-------|
| KE0701 | 114.187 | 234.173 | 420.569 |         | 2.81  |
| KE0702 | 114.187 | 240.669 | 417.259 |         | 2.50  |
| KE0710 | 114.187 |         | 406.531 |         |       |
| KE0720 | 114.187 | 204.183 | 396.818 |         | 2.73  |
| KE0725 | 128.171 |         |         |         |       |
| KE0730 | 128.171 |         |         |         |       |
| KE0735 | 142.154 |         |         |         |       |
| KE0740 | 112.171 |         | 453.558 |         | 3.10  |
| KE0745 | 112.171 | 259.258 |         |         |       |
| KE0746 | 112.171 | 199.683 |         |         |       |
| KE0747 | 112.171 | 232.574 |         |         |       |
| KE0760 | 122.123 | 340.141 |         |         |       |
| KE0800 | 128.214 | 252.862 | 446.425 |         | 2.72  |
| KE0801 | 128.214 |         | 440.863 |         |       |
| KE0802 | 128.214 |         |         |         |       |
| KE0810 | 128.214 |         | 428.531 |         |       |
| KE0830 | 128.214 |         | 418.732 |         |       |
| KE0850 | 128.214 | 244.147 | 408.131 |         |       |
| KE0870 | 126.198 |         |         |         |       |
| KE0890 | 126.198 | 317.350 | 474.612 |         | 2.96  |
| KE0910 | 126.198 | 204.933 | 456.335 |         |       |
| KE0930 | 140.182 |         |         |         |       |
| KE0950 | 120.151 | 292.742 | 475.020 |         | 2.96  |
| KE0980 | 154.596 | 291.543 | 510.208 |         | 2.34  |
| KE1000 | 142.241 | 265.654 | 468.465 |         |       |
| KE1001 | 142.241 |         |         |         |       |
| KE1002 | 142.241 |         |         |         |       |
| KE1003 | 142.241 | 267.253 | 461.590 | 640.000 | 2.320 |
| KE1020 | 142.241 | 227.137 | 441.414 |         | 2.66  |
| KE1040 | 142.241 | 247.925 | 426.700 |         | 2.64  |
| KE1060 | 140.225 |         |         |         |       |
| KE1100 | 140.225 | 305.050 | 493.570 |         | 2.85  |
| KE1150 | 138.209 | 301.141 | 470.391 |         | 2.38  |
| KE1180 | 134.177 | 291.753 | 490.914 |         | 2.88  |
| KE1181 | 134.177 | 257.759 |         |         | 2.72  |
| KE1200 | 134.177 |         | 497.474 |         | 3.23  |
| KE1250 | 132.162 |         |         |         | 3.41  |
| KE1320 | 156.224 |         |         |         |       |
| KE1350 | 296.001 | 305.140 |         |         |       |
| KE1360 | 207.099 |         |         |         |       |
| KE1400 | 156.267 | 276.248 | 483.296 |         |       |
| KE1401 | 156.267 |         |         |         |       |
| KE1403 | 156.267 |         |         |         |       |
| KE1500 | 154.252 | 295.950 |         |         | 2.75  |
| KE1530 | 154.252 | 266.603 |         |         | 2.83  |
| KE1550 | 154.252 |         |         |         |       |
| KE1580 | 152.236 |         |         |         |       |
| KE1600 | 152.236 | 278.147 | 466.413 |         | 2.93  |
| KE1620 | 152.236 | 452.683 | 480.706 |         | 2.98  |
| KE1640 | 152.236 |         | 474.193 |         |       |
| KE1660 | 152.236 |         |         |         |       |

Table 7. Compound constant values--Continued

|        |         |         |         |      |
|--------|---------|---------|---------|------|
| KE1680 | 152.236 |         |         |      |
| KE1700 | 150.220 | 502.086 |         |      |
| KE1720 | 146.188 |         |         |      |
| KE1750 | 148.204 | 502.000 |         | 2.83 |
| KE1760 | 148.204 |         |         |      |
| KE1762 | 148.204 |         |         |      |
| KE1800 | 148.204 |         |         |      |
| KE1820 | 148.204 |         |         |      |
| KE1821 | 148.204 | 248.914 |         |      |
| KE1860 | 162.188 | 331.640 |         |      |
| KE1900 | 162.188 | 303.640 |         |      |
| KE1901 | 162.188 | 386.655 |         | 2.74 |
| KE2000 | 247.131 |         |         |      |
| KE2100 | 170.294 | 285.944 | 506.295 | 2.70 |
| KE2104 | 170.294 | 287.744 | 500.554 | 2.68 |
| KE2120 | 168.278 |         |         |      |
| KE2130 | 196.246 |         |         |      |
| KE2150 | 162.231 | 264.155 |         |      |
| KE2155 | 162.231 |         |         |      |
| KE2170 | 160.215 |         |         |      |
| KE2190 | 275.142 |         |         |      |
| KE2225 | 182.305 | 335.550 | 549.670 | 2.75 |
| KE2235 | 182.305 |         |         |      |
| KE2250 | 176.258 | 300.141 | 538.400 |      |
| KE2260 | 170.210 |         | 568.721 |      |
| KE2261 | 170.210 | 328.640 | 573.150 |      |
| KE2300 | 198.348 | 300.641 | 541.172 |      |
| KE2330 | 192.300 |         | 523.204 |      |
| KE2331 | 192.300 |         |         | 3.50 |
| KE2350 | 190.285 | 290.143 | 544.516 |      |
| KE2365 | 182.221 | 320.989 | 579.097 | 2.98 |
| KE2380 | 184.237 |         | 579.223 |      |
| KE2430 | 210.232 | 368.148 | 620.160 | 3.71 |
| KE2445 | 198.264 |         |         |      |
| KE2460 | 208.216 | 558.019 | 649.984 |      |
| KE2473 | 240.215 | 467.190 | 723.129 |      |
| KE2474 | 240.215 |         |         |      |
| KE2477 | 240.215 |         |         |      |
| KE2506 | 226.401 | 312.389 | 567.786 | 2.73 |
| KE2540 | 218.338 | 287.144 |         |      |
| KE2545 | 210.275 | 307.640 | 604.154 | 2.81 |
| KE2565 | 212.291 |         |         |      |
| KE2630 | 258.316 |         |         |      |
| KE2645 | 226.318 |         |         |      |
| KE2680 | 323.229 |         |         |      |
| KE2685 | 402.125 |         |         |      |
| KE2688 | 337.213 |         |         |      |
| KE2707 | 254.455 | 326.139 |         | 2.40 |
| KE2745 | 234.297 | 385.154 |         | 3.30 |
| KE2755 | 240.344 |         |         |      |
| KE2775 | 230.265 | 447.181 |         | 3.41 |

Table 7. Compound constant values--Continued

|        |         |         |      |
|--------|---------|---------|------|
| KE2835 | 260.419 | 317.639 |      |
| KE2845 | 254.371 |         |      |
| KE3050 | 288.472 | 325.639 |      |
| KE3310 | 338.616 | 342.441 | 2.50 |
| KE3350 | 316.526 | 332.140 |      |
| KE3712 | 394.723 | 350.343 | 2.32 |
| KE4114 | 450.830 | 356.844 |      |
| KE4516 | 506.937 | 361.846 |      |

### 5.1.2. Melting Point

Melting and freezing point values were transcribed along with the other properties and listed by program CONCON. However, the values selected for tabulation in Table 7 were usually obtained from the TRC Tables [3270]. A value from another source was used only in those few instances when a high-quality value published later than the TRC table appeared to provide better information. No attempt was made to apply any external checks to the melting point values, such as plotting the values for homologs versus carbon number. No distinction was made between freezing and melting point values; both are listed in Table 7 as melting point (MP) values.

A few triple point values were found in the literature but more often than not the relation to the corresponding melting point appeared anomalous. Hence the decision not to include the triple point values in Table 7.

### 5.1.3. Normal Boiling Point

As explained in section 4.1 and 4.2.3, the normal boiling point values listed in Table 7 are those calculated from the final vapor pressure fits for either range 2 or range 4. Table 8 shows how the final selected values differ from the ketone values given in Ambrose [10318, 41765] and the TRC tables [3270]. When normal boiling point values appeared in Ambrose [41765], they were chosen as the tentative selected values and used as a guideline in the vapor pressure data fitting, hence our values are biased toward the Ambrose values.

Table 8. Comparison of selected normal boiling points with those of other compilations

| Compound | This    | Other compilations |            |
|----------|---------|--------------------|------------|
|          | report  | Ambrose [41765]    | TRC [3270] |
| KE0300   | 329.207 | 329.200            | 329.429    |
| KE0400   | 352.747 | 352.740            | 352.784    |
| KE0500   | 375.408 | 375.410            | 375.460    |
| KE0501   | 375.109 | 375.110            | 375.140    |
| KE0505   | 367.482 | 367.480            | 367.548    |
| KE0600   | 400.733 | 400.700            | 400.860    |
| KE0601   | 396.656 | 396.600            | 396.658    |
| KE0604   | 388.856 | 389.600            | 389.656    |
| KE0605   | 388.032 |                    | 386.554    |
| KE0607   | 379.263 | 379.263 [10318]    | 379.452    |
| KE0620   | 428.763 | 428.900            |            |
| KE0700   | 424.206 | 424.200            | 424.070    |
| KE0701   | 420.569 |                    | 420.569    |
| KE0702   | 417.259 |                    | 417.167    |
| KE0710   | 406.531 |                    | 406.163    |
| KE0720   | 396.818 |                    | 397.559    |
| KE0800   | 446.425 |                    | 445.780    |
| KE1000   | 468.465 |                    | 467.490    |
| KE1400   | 483.296 |                    | 483.296    |
| KE2100   | 506.295 | 506.300 [10318]    | 501.103    |
| KE2300   | 541.172 | 541.200 [10318]    | 536.215    |

In Table 8, the differences between the final selected values and those listed by Ambrose or the TRC tables are large enough to merit discussion for seven compounds: KE0605, KE0710, KE0720, KE0800, KE1000, KE2100 and KE2300.

For KE0605, the input to program CONCON included three normal boiling point values besides the value from the TRC table. Those values were 387.655 from Bryant et al. [8181], 388.255 from Ginnings et al. [13065] and 388.155 from Jamison et al. [21544]. All three were retained for the final correlation along with 9 points from Loginova et al. [15776] over the range from 300.15 to 382.15. Hence, all the information found supports the 388.032 K value rather than the lower TRC value.

No normal boiling point values were found for KE0710. The only vapor pressure data found was an equation from Mayberry and Aston [13799] which gave 406.531 for the normal boiling point. There is no particular reason to believe that value is any better than the 406.163 K value given by the TRC tables.

For KE0720, 10 normal boiling point values were found in the literature and those values scattered around the TRC value of 397.55. Our vapor pressure correlation is based upon points calculated from the equation of Mayberry and Aston [13799] over the range 350 to 440 K, and on points from Dreisbach and Shrader [1361] from 293 to 344 K. The Dreisbach and Shrader value for the normal boiling point was 398.409 whereas the Mayberry and Aston equation gives 396.818. The Mayberry et al. vapor pressure data were chosen over the Driesbach et al. data in the 350 to 400 K range, primarily because the latter ended at the normal boiling point while the former could be extrapolated (rightly or wrongly) above the normal boiling point. The true normal boiling point probably lies between the Mayberry et al. and the Driesbach et al. values in the vicinity of the 397.559 value given by the TRC tables.

With the exception of two values which were about 3 K below all the other values, all other literature values retrieved (six of them) for the normal boiling point of KE0800 were above 446 K. The final vapor pressure correlations were based on the vapor pressure data of Geisler and Ratzsch [18439] and the boiling point values reported by Deffet [5736] (446.681 K), Bruhl [5842] (100.352 kPa at 446.080 K), Ceuterick [9712] (100.658 kPa at 446.180 K), Mironenko et al. [15791] (446.250 K) and Lecat [21283] (446.030 K). It is believed that the TRC table value is slightly low for KE0800.

For KE2100 and KE2300, the more recent data of Ambrose et al. [10318] supersedes the older TRC values.

#### 5.1.4. Critical Properties

Values for one or more critical properties were found for 14 compounds: KE0300, KE0370, KE0380, KE0400, KE0500, KE0501, KE0505, KE0600, KE0601, KE0604, KE0607, KE0620, KE0700, and KE1003. Ambrose [41765] lists selected values for all of these compounds except for the two halogenated ketones KE0370 and KE0380. No reason was found to change the values selected by Ambrose.

The compilation of Kudchadker, Alani and Zwolinski [1051] lists the  $T_c$  and  $P_c$  values of Murphy [10015] for KE0370. Those values are evidently the only existing ones. Also, the only vapor pressure data set for KE0370 is from Murphy.

Kudchadker et al. also selected Murphy's [10015]  $T_c$  and  $P_c$  values for KE0380 because they were the only values available at the time. The values which have appeared since then are listed below with Murphy's values.

|                                  | <u>T<sub>c</sub>, K</u> | <u>P<sub>c</sub>, MPa</u> |
|----------------------------------|-------------------------|---------------------------|
| Murphy [10015]                   | 357.245                 | 2.841                     |
| Plaush and Pace [15034]          | 357.245                 | 2.834                     |
| Glowka and Zawisza [16255]       | 357.185                 | 2.837                     |
| Mousa, Kay and Kreglewski [7465] | 357.135                 | 2.832                     |
| Mousa [40009]                    | 357.135                 | 2.832                     |

The values of Mousa [40009] were selected initially. However, the Murphy  $T_c$  and  $P_c$  values worked a little better with the available vapor pressure values near the critical point and were chosen as the final selected values.

When  $P_c$ ,  $T_c$  and  $V_c$  were all available,  $Z_c$  was calculated using  
 $R = 0.00831441 \text{ MPa cm}^3/\text{mol K}$ .

#### 5.1.5. Acentric Factor

The acentric factor was calculated for every compound with  $T_c$  and  $P_c$  values. The calculation was automatically done by program PFIT for every vapor pressure fit. The acentric factor value selected for the compound was the one from the correlation used to calculate the final normal boiling point if  $T_r = 0.7$  fell within the temperature range of that correlation. In some instances when the normal boiling point was obtained from the range 2 fit, it was necessary to use the acentric factor from the range 4 fit because  $T_r = 0.7$  fell outside range 2.

In the case of KE0601, due to limited data, the last selected data point (besides the critical point) fell 1.35 K short of  $T_r = 0.7$ , and for that compound the acentric factor was calculated from a correlation equation which was extrapolated by that amount. This was the only one of the 14 acentric factors whose calculation involved an extrapolation of the vapor pressure data.

#### 5.1.6. Dipole Moment

The number of literature articles reporting dipole moments is large. Most of that literature was retrieved for the data evaluation program because dipole moment data usually involve binary density data. Unfortunately, the processing and evaluation of the dipole moment data is beyond the scope of our evaluation effort, and no attempt was made to process the literature dipole moment data.

The dipole moment is an important property for physical property correlations, e.g., correlations for the second virial coefficient. As a convenience for the users of this report, dipole moment values from McClellan [5266] have been included in Table 7. When McClellan listed a recommended value for a compound, that value was used. When no recommended value was listed, the values in Table 7 were obtained by taking an arithmetic average of the literature values for solvent measurements listed by McClellan. Any values listed for the pure gas or pure liquid were excluded from the averaging.

#### 5.1.7. Radius of Gyration

Like the dipole moment, the radius of gyration is often used in physical property correlations. As a convenience to the user, values from Thompson [1706] are listed in Table 7. No attempt was made to check or extend the Thompson values.

## 5.2. Vapor Pressure

The vapor pressure correlation constants for the range 1, 2, 3 and 4 fits are listed in tables 9, 10, 11 and 12 respectively. There are two lines for each correlation, and the compound's identification number appears at the beginning of each line.

The first item following the identification number on the first line for each compound is a single letter--from A through K--which characterizes the quality of the experimental data base for the correlation. Before discussing the vapor pressure correlations in tables 9 through 12, it is necessary to define the quality ratings and give the reader some insight as to how they have been used for both the vapor pressure and liquid density correlations.

Table 9. Range 1 vapor pressure correlations

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE0300 | A 102           | WAGNER** | -0.74974490D 01 | 0.13173750D 01  | -0.26754153D 01  |
| KE0300 | -0.26773997D 01 |          | 0.50809985D 03  | 0.46999960D 01  | 247 509 0.10D 01 |
| KE0305 | I 12            | RPM2**** | 0.51708912D 02  | -0.74019867D 04 | -0.11732730D 00  |
| KE0305 | 0.12983094D-03  |          |                 |                 | 238 294 0.18D-01 |
| KE0360 | I 4             | RPM2**** | 0.63297187D 02  | -0.10289174D 05 | -0.13078063D 00  |
| KE0360 | 0.12264536D-03  |          |                 |                 | 303 392 0.46D-03 |
| KE0361 | I 4             | RPM2**** | 0.26169771D 02  | -0.55232119D 04 | -0.28809006D-01  |
| KE0361 | 0.24994206D-04  |          |                 |                 | 292 392 0.38D-03 |
| KE0362 | J 5             | RPM2**** | 0.43814304D 01  | -0.42660432D 04 | 0.37510628D-01   |
| KE0362 | -0.34712350D-04 |          |                 |                 | 348 446 0.33D-01 |
| KE0370 | I 17            | RIEDEL** | 0.52021099D 02  | -0.55057334D 01 | -0.46044849D 04  |
| KE0370 | 0.60184321D-16  |          |                 |                 | 232 411 0.72D 00 |
| KE0380 | G 35            | WAGNER** | -0.76569653D 01 | 0.12828020D 01  | -0.39738249D 01  |
| KE0380 | -0.72826939D 01 |          | 0.35724463D 03  | 0.28411484D 01  | 194 358 0.29D 01 |
| KE0400 | A 65            | WAGNER** | -0.76980638D 01 | 0.16857248D 01  | -0.35946384D 01  |
| KE0400 | -0.14844025D 01 |          | 0.53677979D 03  | 0.42069960D 01  | 265 537 0.33D 01 |
| KE0410 | J 9             | RPM2**** | -0.36104822D 02 | 0.79123257D 03  | 0.17481982D 00   |
| KE0410 | -0.18881169D-03 |          |                 |                 | 260 363 0.33D 00 |
| KE0420 | H 16            | RPM2**** | 0.19664233D 02  | -0.49770013D 04 | -0.31815092D-02  |
| KE0420 | -0.34876835D-05 |          |                 |                 | 249 381 0.84D-01 |
| KE0430 | K 2             | RPM2**** | 0.16936190D 02  | -0.49228300D 04 | 0.00000000D 00   |
| KE0430 | 0.00000000D 00  |          |                 |                 | 343 400          |
| KE0440 | J 6             | RPM2**** | -0.25859342D 03 | 0.25691015D 05  | 0.84404370D 00   |
| KE0440 | -0.86319912D-03 |          |                 |                 | 300 355 0.64D 00 |
| KE0445 | J 13            | RPM2**** | -0.37836491D 03 | 0.46708999D 05  | 0.10059766D 01   |
| KE0445 | -0.85404877D-03 |          |                 |                 | 372 416 0.85D 00 |
| KE0446 | K 2             | RPM2**** | 0.17404000D 02  | -0.58193928D 04 | 0.00000000D 00   |
| KE0446 | 0.00000000D 00  |          |                 |                 | 343 456          |
| KE0450 | J 9             | RPM2**** | 0.68041358D 02  | -0.12469551D 05 | -0.12079499D 00  |
| KE0450 | 0.95103685D-04  |          |                 |                 | 322 428 0.80D-01 |
| KE0451 | J 8             | RPM2**** | 0.11101456D 03  | -0.16741801D 05 | -0.25145797D 00  |
| KE0451 | 0.22344785D-03  |          |                 |                 | 306 410 0.90D-01 |
| KE0460 | I 17            | RPM2**** | 0.16738657D 02  | -0.46777777D 04 | -0.33828305D-03  |
| KE0460 | 0.29316526D-06  |          |                 |                 | 309 391 0.18D-03 |
| KE0500 | E 37            | WAGNER** | -0.73516670D 01 | 0.58891876D 00  | -0.21522346D 01  |
| KE0500 | -0.58445133D 01 |          | 0.56107983D 03  | 0.36939983D 01  | 282 545 0.26D 01 |
| KE0501 | E 40            | WAGNER** | -0.70827199D 01 | 0.21564015D 00  | -0.25715917D 01  |
| KE0501 | -0.24178698D 01 |          | 0.56145996D 03  | 0.37289982D 01  | 282 545 0.37D 01 |
| KE0505 | E 34            | WAGNER** | -0.72049532D 01 | 0.35067807D 00  | -0.13709136D 01  |
| KE0505 | -0.75396462D 01 |          | 0.55339990D 03  | 0.38499985D 01  | 276 550 0.45D 01 |
| KE0510 | H 29            | RPM2**** | -0.48963358D 02 | 0.24378665D 04  | 0.19501662D 00   |
| KE0510 | -0.19254584D-03 |          |                 |                 | 289 412 0.17D 00 |
| KE0520 | I 28            | VAPRES-2 | 0.24376810D 03  | -0.11456854D 05 | 0.75261551D-01   |
| KE0520 | -0.24333219D-04 |          | -0.39526822D 02 |                 | 273 539 0.12D 01 |
| KE0530 | J 6             | RPM2**** | 0.16466401D 02  | -0.45368554D 04 | -0.35654411D-03  |
| KE0530 | 0.31524389D-06  |          |                 |                 | 355 380 0.00D 00 |
| KE0540 | J 5             | RPM2**** | -0.11112349D 03 | 0.10130898D 05  | 0.37424566D 00   |
| KE0540 | -0.36622482D-03 |          |                 |                 | 311 371 0.16D 00 |
| KE0555 | I 13            | RPM2**** | 0.17581976D 02  | -0.54557925D 04 | -0.54307219D-03  |
| KE0555 | 0.48989525D-06  |          |                 |                 | 272 333 0.11D-04 |

Table 9. Range 1 vapor pressure correlations--Continued

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE0563 | I 5             | RPM2**** | -0.36593305D 02 | 0.11972196D 04  | 0.13428023D 00   |
| KE0563 | -0.10980973D-03 |          |                 |                 | 382 463 0.77D-02 |
| KE0565 | I 14            | RPM2**** | 0.20595620D 02  | -0.56476721D 04 | -0.66797188D-02  |
| KE0565 | 0.21173870D-05  |          |                 |                 | 317 419 0.18D 00 |
| KE0566 | I 8             | RPM2**** | 0.41970324D 02  | -0.99808633D 04 | -0.52226934D-01  |
| KE0566 | 0.39833865D-04  |          |                 |                 | 317 459 0.85D-01 |
| KE0570 | I 11            | RPM2**** | 0.31404936D 02  | -0.87815700D 04 | -0.32014182D-01  |
| KE0570 | 0.34129310D-04  |          |                 |                 | 277 333 0.13D-04 |
| KE0600 | C 32            | WAGNER** | -0.81315482D 01 | 0.18766746D 01  | -0.42287461D 01  |
| KE0600 | -0.27338595D 01 |          | 0.58700000D 03  | 0.33229990D 01  | 298 428 0.38D-02 |
| KE0601 | C 24            | WAGNER** | -0.79647906D 01 | 0.17198839D 01  | -0.42568912D 01  |
| KE0601 | -0.23051546D 01 |          | 0.58281982D 03  | 0.33199987D 01  | 298 407 0.35D-02 |
| KE0604 | H 29            | RIEDEL** | 0.60863450D 02  | -0.64833400D 01 | -0.68459575D 04  |
| KE0604 | 0.10731339D-16  |          |                 |                 | 283 567 0.18D 01 |
| KE0605 | J 12            | RPM2**** | 0.67406874D 02  | -0.11369426D 05 | -0.12515635D 00  |
| KE0605 | 0.10012928D-03  |          |                 |                 | 300 389 0.52D 00 |
| KE0607 | C 38            | WAGNER** | -0.76569055D 01 | 0.16102765D 01  | -0.36188184D 01  |
| KE0607 | -0.28748554D 01 |          | 0.56700000D 03  | 0.34699984D 01  | 284 406 0.71D-02 |
| KE0620 | H 32            | WAGNER** | -0.82635171D 01 | 0.91380629D 00  | -0.57455934D-01  |
| KE0620 | -0.10049146D 02 |          | 0.62900000D 03  | 0.38499985D 01  | 302 582 0.63D 01 |
| KE0640 | I 13            | RPM2**** | 0.12562638D 02  | -0.42869180D 04 | 0.11158413D-01   |
| KE0640 | -0.10948396D-04 |          |                 |                 | 401 561 0.15D 01 |
| KE0645 | I 4             | RPM2**** | 0.41406877D 02  | -0.79886545D 04 | -0.61649738D-01  |
| KE0645 | 0.49977846D-04  |          |                 |                 | 273 395 0.49D-03 |
| KE0650 | J 13            | RPM2**** | 0.40684782D 01  | -0.37767853D 04 | 0.45759886D-01   |
| KE0650 | -0.52451646D-04 |          |                 |                 | 287 404 0.13D 00 |
| KE0660 | J 8             | RIEDEL** | 0.46007514D 04  | -0.67240180D 03 | -0.23440132D 06  |
| KE0660 | 0.41021702D-14  |          |                 |                 | 392 402 0.25D-01 |
| KE0670 | H 15            | RPM2**** | 0.21864140D 02  | -0.64159922D 04 | -0.77320691D-02  |
| KE0670 | 0.36538030D-05  |          |                 |                 | 310 442 0.21D-02 |
| KE0680 | I 4             | RPM2**** | -0.53089226D 02 | 0.31022259D 04  | 0.17381281D 00   |
| KE0680 | -0.14074304D-03 |          |                 |                 | 377 488 0.20D-02 |
| KE0700 | F 46            | WAGNER** | -0.99483801D 01 | 0.47053877D 01  | -0.67889499D 01  |
| KE0700 | -0.17144393D 00 |          | 0.61150000D 03  | 0.34359989D 01  | 274 453 0.60D-01 |
| KE0702 | I 7             | RPM2**** | 0.12619969D 02  | -0.44925265D 04 | 0.11623943D-01   |
| KE0702 | -0.11975873D-04 |          |                 |                 | 273 418 0.13D-01 |
| KE0710 | I 11            | RPM2**** | 0.16894049D 02  | -0.49772008D 04 | -0.12070011D-03  |
| KE0710 | 0.99568801D-07  |          |                 |                 | 349 451 0.66D-03 |
| KE0720 | H 15            | VAPRES-2 | 0.47099357D 03  | -0.15989232D 05 | 0.19827006D 00   |
| KE0720 | -0.79336319D-04 |          | -0.82270805D 02 |                 | 293 441 0.26D-01 |
| KE0740 | I 22            | RPM2**** | 0.30238353D 02  | -0.75018223D 04 | -0.28252855D-01  |
| KE0740 | 0.18152509D-04  |          |                 |                 | 313 465 0.31D-01 |
| KE0800 | I 12            | RPM2**** | -0.58281733D 02 | 0.46022852D 04  | 0.19032262D 00   |
| KE0800 | -0.16244189D-03 |          |                 |                 | 293 447 0.13D 00 |
| KE0801 | I 11            | RPM2**** | -0.16377240D 02 | -0.14125767D 04 | 0.91139663D-01   |
| KE0801 | -0.82220634D-04 |          |                 |                 | 293 441 0.13D 00 |
| KE0802 | J 12            | RPM2**** | 0.51574275D 02  | -0.86523422D 04 | -0.10643159D 00  |
| KE0802 | 0.10186297D-03  |          |                 |                 | 288 424 0.19D 00 |
| KE0810 | I 11            | RPM2**** | 0.16856127D 02  | -0.52338853D 04 | -0.88892330D-04  |
| KE0810 | 0.75498105D-07  |          |                 |                 | 380 481 0.64D-03 |
| KE0830 | J 11            | RPM2**** | 0.16867186D 02  | -0.51189412D 04 | -0.88156709D-04  |
| KE0830 | 0.73679066D-07  |          |                 |                 | 359 461 0.45D-03 |

Table 9. Range 1 vapor pressure correlations--Continued

|        |                 |           |                 |                 |                  |
|--------|-----------------|-----------|-----------------|-----------------|------------------|
| KE0850 | I 8             | RPM2***** | 0.33729517D 02  | -0.82632914D 04 | -0.30963951D-01  |
| KE0850 | 0.22649922D-04  |           |                 |                 | 287 409 0.59D-01 |
| KE0870 | I 11            | RPM2***** | 0.17090378D 02  | -0.55896563D 04 | -0.45415371D-03  |
| KE0870 | 0.39330977D-06  |           |                 |                 | 279 381 0.21D-04 |
| KE0890 | I 13            | RPM2***** | 0.22435782D 02  | -0.67642090D 04 | -0.84645315D-02  |
| KE0890 | 0.20066396D-05  |           |                 |                 | 394 485 0.39D-01 |
| KE0910 | I 4             | RIEDEL**  | 0.23473348D 04  | -0.34498341D 03 | -0.11554548D 06  |
| KE0910 | 0.25357439D-14  |           |                 |                 | 332 457 0.76D-05 |
| KE0950 | G 58            | VAPRES-2  | -0.26240368D 04 | 0.50707528D 05  | -0.13624744D 01  |
| KE0950 | 0.60820529D-03  |           | 0.49191888D 03  |                 | 303 476 0.16D 00 |
| KE0980 | J 7             | RPM2***** | 0.63746621D 02  | -0.13829575D 05 | -0.95899972D-01  |
| KE0980 | 0.64946645D-04  |           |                 |                 | 415 511 0.42D-01 |
| KE1000 | I 23            | VAPRES-2  | 0.25066182D 04  | -0.66711165D 05 | 0.11440382D 01   |
| KE1000 | -0.48792265D-03 |           | -0.45344764D 03 |                 | 333 469 0.35D-01 |
| KE1003 | C 31            | WAGNER**  | -0.86650883D 01 | 0.18886549D 01  | -0.55050132D 01  |
| KE1003 | -0.29487241D 01 |           | 0.64000000D 03  | 0.23199987D 01  | 298 486 0.79D-02 |
| KE1020 | I 13            | VAPRES-2  | 0.40176615D 03  | -0.17039623D 05 | 0.12875484D 00   |
| KE1020 | -0.44344156D-04 |           | -0.66788250D 02 |                 | 333 454 0.10D-02 |
| KE1060 | I 11            | RPM2***** | 0.17107479D 02  | -0.58037434D 04 | -0.41235569D-03  |
| KE1060 | 0.35515840D-06  |           |                 |                 | 299 401 0.34D-04 |
| KE1100 | I 18            | RPM2***** | 0.42065341D 02  | -0.96075335D 04 | -0.56094570D-01  |
| KE1100 | 0.39838002D-04  |           |                 |                 | 333 494 0.73D-03 |
| KE1180 | I 7             | RPM2***** | -0.31931183D 02 | 0.76175152D 03  | 0.11630691D 00   |
| KE1180 | -0.91697854D-04 |           |                 |                 | 405 491 0.56D-01 |
| KE1200 | I 17            | RPM2***** | 0.17973910D 02  | -0.63745665D 04 | -0.17194104D-02  |
| KE1200 | 0.12669434D-05  |           |                 |                 | 369 521 0.85D-02 |
| KE1500 | I 15            | RPM2***** | 0.44285192D 02  | -0.10504622D 05 | -0.57468922D-01  |
| KE1500 | 0.39224351D-04  |           |                 |                 | 353 424 0.20D-03 |
| KE1600 | I 16            | RPM2***** | 0.16332197D 02  | -0.54509453D 04 | -0.94791231D-04  |
| KE1600 | 0.79497020D-07  |           |                 |                 | 369 521 0.66D-03 |
| KE1620 | H 21            | RPM2***** | -0.73204088D 02 | 0.90466559D 04  | 0.18287068D 00   |
| KE1620 | -0.12508377D-03 |           |                 |                 | 451 500 0.33D 00 |
| KE1700 | I 16            | RPM2***** | 0.17009724D 02  | -0.62063641D 04 | -0.10441452D-03  |
| KE1700 | 0.87991144D-07  |           |                 |                 | 369 521 0.32D-03 |
| KE1720 | I 20            | RPM2***** | 0.99367506D 02  | -0.19759721D 05 | -0.17211686D 00  |
| KE1720 | 0.11966357D-03  |           |                 |                 | 375 535 0.44D-02 |
| KE1800 | K 2             | RPM2***** | 0.15630510D 02  | -0.58530705D 04 | 0.00000000D 00   |
| KE1800 | 0.00000000D 00  |           |                 |                 | 395 403          |
| KE1820 | J 11            | RPM2***** | 0.25265859D 02  | -0.47381032D 04 | -0.49092128D-01  |
| KE1820 | 0.47445496D-04  |           |                 |                 | 292 417 0.26D-01 |
| KE1821 | J 8             | RPM2***** | -0.83424914D 02 | 0.52538877D 04  | 0.31324636D 00   |
| KE1821 | -0.33243093D-03 |           |                 |                 | 294 368 0.30D-01 |
| KE1900 | J 5             | RPM2***** | -0.99897398D 02 | 0.12670804D 05  | 0.23088809D 00   |
| KE1900 | -0.14890088D-03 |           |                 |                 | 323 418 0.13D-01 |
| KE1901 | J 8             | RPM2***** | 0.66819317D 04  | -0.92881114D 06 | -0.16059749D 02  |
| KE1901 | 0.12896429D-01  |           |                 |                 | 388 431 0.26D-01 |
| KE2100 | F 35            | RPM2***** | 0.39808738D 02  | -0.10382444D 05 | -0.40885275D-01  |
| KE2100 | 0.23468422D-04  |           |                 |                 | 298 539 0.36D-01 |
| KE2104 | C 32            | VAPRES-2  | 0.38789128D 03  | -0.19284923D 05 | 0.10027672D 00   |
| KE2104 | -0.29008985D-04 |           | -0.62369530D 02 |                 | 298 532 0.12D-01 |
| KE2120 | I 7             | RPM2***** | -0.43389210D 02 | 0.30307622D 04  | 0.12861987D 00   |
| KE2120 | -0.92236652D-04 |           |                 |                 | 449 501 0.10D-01 |

Table 9. Range 1 vapor pressure correlations--Continued

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE2225 | I 23            | VAPRES-2 | -0.30334436D 03 | -0.12188523D 03 | -0.14965503D 00  |
| KE2225 | 0.56469159D-04  |          | 0.59179741D 02  |                 | 408 564 0.18D-01 |
| KE2261 | K 2             | RPM2**** | 0.19418350D 02  | -0.84826264D 04 | 0.00000000D 00   |
| KE2261 | 0.00000000D 00  |          |                 |                 | 417 574          |
| KE2300 | F 19            | VAPRES-2 | -0.62855974D 03 | 0.57720465D 04  | -0.31642310D 00  |
| KE2300 | 0.12610738D-03  |          | 0.12024952D 03  |                 | 333 542 0.53D-01 |
| KE2330 | J 10            | RPM2**** | 0.44650283D 02  | -0.11158370D 05 | -0.57059059D-01  |
| KE2330 | 0.40726555D-04  |          |                 |                 | 286 524 0.10D-01 |
| KE2331 | J 10            | RPM2**** | -0.19575553D 04 | 0.19631481D 06  | 0.63736451D 01   |
| KE2331 | -0.68379550D-02 |          |                 |                 | 291 330 0.25D-03 |
| KE2365 | G 45            | VAPRES-2 | -0.73382832D 03 | 0.11307120D 05  | -0.29425735D 00  |
| KE2365 | 0.10027145D-03  |          | 0.13451238D 03  |                 | 329 622 0.30D 00 |
| KE2460 | J 26            | RIEDEL** | 0.36652016D 03  | -0.48575010D 02 | -0.32112042D 05  |
| KE2460 | 0.28048558D-16  |          |                 |                 | 558 651 0.31D 00 |
| KE2473 | J 7             | RPM2**** | -0.22362756D 01 | -0.64738203D 04 | 0.43962829D-01   |
| KE2473 | -0.30566467D-04 |          |                 |                 | 474 724 0.38D-01 |
| KE2474 | J 22            | RPM2**** | 0.18832730D 03  | -0.38592193D 05 | -0.36089778D 00  |
| KE2474 | 0.26967276D-03  |          |                 |                 | 410 496 0.10D-02 |
| KE2477 | J 20            | RPM2**** | -0.35975370D 00 | -0.10541719D 05 | 0.76920902D-01   |
| KE2477 | -0.68264351D-04 |          |                 |                 | 373 457 0.51D-03 |
| KE2506 | C 16            | RPM2**** | 0.50594333D 02  | -0.13634600D 05 | -0.56890913D-01  |
| KE2506 | 0.32071991D-04  |          |                 |                 | 437 601 0.51D 00 |
| KE2545 | I 39            | RIEDEL** | 0.73424260D 02  | -0.76018739D 01 | -0.12094587D 05  |
| KE2545 | -0.21751014D-17 |          |                 |                 | 503 604 0.15D 00 |
| KE2775 | J 9             | RPM2**** | 0.54175963D 03  | -0.10033771D 06 | -0.10049879D 01  |
| KE2775 | 0.63820178D-03  |          |                 |                 | 456 549 0.12D-01 |
| KE3350 | K 2             | RPM2**** | 0.28106180D 02  | -0.14368583D 05 | 0.00000000D 00   |
| KE3350 | 0.00000000D 00  |          |                 |                 | 443 525          |

Table 10. Range 2 vapor pressure correlations

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE0300 | A 79            | WAGNER** | -0.75475020D 01 | 0.14452612D 01  | -0.29036443D 01  |
| KE0300 | -0.21275823D 01 |          | 0.50809985D 03  | 0.46999960D 01  | 247 348 0.28D-01 |
| KE0305 | I 12            | RPM2**** | 0.51708912D 02  | -0.74019867D 04 | -0.11732730D 00  |
| KE0305 | 0.12983094D-03  |          |                 |                 | 238 294 0.18D-01 |
| KE0360 | I 4             | RPM2**** | 0.63297187D 02  | -0.10289174D 05 | -0.13078063D 00  |
| KE0360 | 0.12264536D-03  |          |                 |                 | 303 392 0.46D-03 |
| KE0361 | I 4             | RPM2**** | 0.26169771D 02  | -0.55232119D 04 | -0.28809006D-01  |
| KE0361 | 0.24994206D-04  |          |                 |                 | 292 392 0.38D-03 |
| KE0362 | J 5             | RPM2**** | 0.43814304D 01  | -0.42660432D 04 | 0.37510628D-01   |
| KE0362 | -0.34712350D-04 |          |                 |                 | 348 446 0.33D-01 |
| KE0370 | I 7             | RIEDEL** | 0.51924067D 02  | -0.54678495D 01 | -0.46277611D 04  |
| KE0370 | -0.94190148D-17 |          |                 |                 | 232 287 0.99D-01 |
| KE0380 | G 15            | WAGNER** | -0.68017611D 01 | -0.90258908D 00 | 0.74037148D-01   |
| KE0380 | -0.18709122D 02 |          | 0.35724463D 03  | 0.28411484D 01  | 194 265 0.21D 00 |
| KE0400 | A 39            | WAGNER** | -0.80361159D 01 | 0.24595576D 01  | -0.46452494D 01  |
| KE0400 | 0.20832996D 00  |          | 0.53677979D 03  | 0.42069960D 01  | 265 371 0.53D-01 |
| KE0410 | J 9             | RPM2**** | -0.36104822D 02 | 0.79123257D 03  | 0.17481982D 00   |
| KE0410 | -0.18881169D-03 |          |                 |                 | 260 363 0.33D 00 |
| KE0420 | H 16            | RPM2**** | 0.19664233D 02  | -0.49770013D 04 | -0.31815092D-02  |
| KE0420 | -0.34876835D-05 |          |                 |                 | 249 381 0.84D-01 |
| KE0430 | K 2             | RPM2**** | 0.16936190D 02  | -0.49228300D 04 | 0.00000000D 00   |
| KE0430 | 0.00000000D 00  |          |                 |                 | 343 400          |
| KE0440 | J 6             | RPM2**** | -0.25859342D 03 | 0.25691015D 05  | 0.84404370D 00   |
| KE0440 | -0.86319912D-03 |          |                 |                 | 300 355 0.64D 00 |
| KE0445 | J 13            | RPM2**** | -0.37836491D 03 | 0.46708999D 05  | 0.10059766D 01   |
| KE0445 | -0.85404877D-03 |          |                 |                 | 372 416 0.85D 00 |
| KE0446 | K 2             | RPM2**** | 0.17404000D 02  | -0.58193928D 04 | 0.00000000D 00   |
| KE0446 | 0.00000000D 00  |          |                 |                 | 343 456          |
| KE0450 | J 9             | RPM2**** | 0.68041358D 02  | -0.12469551D 05 | -0.12079499D 00  |
| KE0450 | 0.95103685D-04  |          |                 |                 | 322 428 0.80D-01 |
| KE0451 | J 8             | RPM2**** | 0.11101456D 03  | -0.16741801D 05 | -0.25145797D 00  |
| KE0451 | 0.22344785D-03  |          |                 |                 | 306 410 0.90D-01 |
| KE0460 | I 17            | RPM2**** | 0.16738657D 02  | -0.46777777D 04 | -0.33828305D-03  |
| KE0460 | 0.29316526D-06  |          |                 |                 | 309 391 0.18D-03 |
| KE0500 | A 25            | WAGNER** | -0.76517516D 01 | 0.13209503D 01  | -0.33462984D 01  |
| KE0500 | -0.32001583D 01 |          | 0.56107983D 03  | 0.36939983D 01  | 282 395 0.29D-01 |
| KE0501 | A 24            | WAGNER** | -0.77760626D 01 | 0.17033533D 01  | -0.41525350D 01  |
| KE0501 | -0.13722948D 01 |          | 0.56145996D 03  | 0.37289982D 01  | 282 385 0.35D-02 |
| KE0505 | B 25            | WAGNER** | -0.79425250D 01 | 0.20530981D 01  | -0.37421557D 01  |
| KE0505 | -0.34919809D 01 |          | 0.55339990D 03  | 0.38499985D 01  | 276 377 0.10D-01 |
| KE0510 | H 29            | RPM2**** | -0.48963358D 02 | 0.24378665D 04  | 0.19501662D 00   |
| KE0510 | -0.19254584D-03 |          |                 |                 | 289 412 0.17D 00 |
| KE0520 | I 17            | VAPRES-2 | 0.56206527D 03  | -0.18068105D 05 | 0.25540648D 00   |
| KE0520 | -0.11377508D-03 |          | -0.99531428D 02 |                 | 273 416 0.31D-01 |
| KE0530 | J 6             | RPM2**** | 0.16466401D 02  | -0.45368554D 04 | -0.35654411D-03  |
| KE0530 | 0.31524389D-06  |          |                 |                 | 355 380 0.00D 00 |
| KE0540 | J 5             | RPM2**** | -0.11112349D 03 | 0.10130898D 05  | 0.37424566D 00   |
| KE0540 | -0.36622482D-03 |          |                 |                 | 311 371 0.16D 00 |
| KE0555 | I 13            | RPM2**** | 0.17581976D 02  | -0.54557925D 04 | -0.54307219D-03  |
| KE0555 | 0.48989525D-06  |          |                 |                 | 272 333 0.11D-04 |
| KE0563 | I 5             | RPM2**** | -0.36593305D 02 | 0.11972196D 04  | 0.13428023D 00   |
| KE0563 | -0.10980973D-03 |          |                 |                 | 382 463 0.77D-02 |

Table 10. Range 2 vapor pressure correlations--Continued

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE0565 | I 14            | RPM2**** | 0.20595620D 02  | -0.56476721D 04 | -0.66797188D-02  |
| KE0565 | 0.21173870D-05  |          |                 |                 | 317 419 0.18D 00 |
| KE0566 | I 8             | RPM2**** | 0.41970324D 02  | -0.99808633D 04 | -0.52226934D-01  |
| KE0566 | 0.39833865D-04  |          |                 |                 | 317 459 0.85D-01 |
| KE0570 | I 11            | RPM2**** | 0.31404936D 02  | -0.87815700D 04 | -0.32014182D-01  |
| KE0570 | 0.34129310D-04  |          |                 |                 | 277 333 0.13D-04 |
| KE0600 | C 30            | WAGNER** | -0.81216982D 01 | 0.18535284D 01  | -0.41948020D 01  |
| KE0600 | -0.27979991D 01 |          | 0.58700000D 03  | 0.33229990D 01  | 298 417 0.29D-02 |
| KE0601 | C 24            | WAGNER** | -0.79647906D 01 | 0.17198839D 01  | -0.42568912D 01  |
| KE0601 | -0.23051546D 01 |          | 0.58281982D 03  | 0.33199987D 01  | 298 407 0.35D-02 |
| KE0604 | H 11            | WAGNER** | -0.54683310D 01 | -0.42671786D 01 | 0.52946853D 01   |
| KE0604 | -0.22805945D 02 |          | 0.57100000D 03  | 0.32699986D 01  | 283 389 0.84D-01 |
| KE0605 | J 12            | RPM2**** | 0.67406874D 02  | -0.11369426D 05 | -0.12515635D 00  |
| KE0605 | 0.10012928D-03  |          |                 |                 | 300 389 0.52D 00 |
| KE0607 | C 36            | WAGNER** | -0.76403269D 01 | 0.15718952D 01  | -0.35647812D 01  |
| KE0607 | -0.29702606D 01 |          | 0.56700000D 03  | 0.34699984D 01  | 284 395 0.68D-02 |
| KE0620 | H 23            | WAGNER** | -0.10550075D 02 | 0.62701309D 01  | -0.77788104D 01  |
| KE0620 | 0.36400539D 01  |          | 0.62900000D 03  | 0.38499985D 01  | 302 434 0.67D-01 |
| KE0645 | I 4             | RPM2**** | 0.41406877D 02  | -0.79886545D 04 | -0.61649738D-01  |
| KE0645 | 0.49977846D-04  |          |                 |                 | 273 395 0.49D-03 |
| KE0650 | J 13            | RPM2**** | 0.40684782D 01  | -0.37767853D 04 | 0.45759886D-01   |
| KE0650 | -0.52451646D-04 |          |                 |                 | 287 404 0.13D 00 |
| KE0660 | J 8             | RIEDEL** | 0.46007514D 04  | -0.67240180D 03 | -0.23440132D 06  |
| KE0660 | 0.41021702D-14  |          |                 |                 | 392 402 0.25D-01 |
| KE0670 | H 15            | RPM2**** | 0.21864140D 02  | -0.64159922D 04 | -0.77320691D-02  |
| KE0670 | 0.36538030D-05  |          |                 |                 | 310 442 0.21D-02 |
| KE0680 | I 4             | RPM2**** | -0.53089226D 02 | 0.31022259D 04  | 0.17381281D 00   |
| KE0680 | -0.14074304D-03 |          |                 |                 | 377 488 0.20D-02 |
| KE0700 | F 44            | WAGNER** | -0.98709446D 01 | 0.45299059D 01  | -0.65596530D 01  |
| KE0700 | -0.50714254D 00 |          | 0.61150000D 03  | 0.34359989D 01  | 274 442 0.39D-01 |
| KE0702 | I 7             | RPM2**** | 0.12619969D 02  | -0.44925265D 04 | 0.11623943D-01   |
| KE0702 | -0.11975873D-04 |          |                 |                 | 273 418 0.13D-01 |
| KE0710 | I 8             | RPM2**** | 0.16968053D 02  | -0.49868283D 04 | -0.30987682D-03  |
| KE0710 | 0.26042134D-06  |          |                 |                 | 349 421 0.36D-03 |
| KE0720 | H 12            | RPM2**** | 0.31024959D 02  | -0.65104600D 04 | -0.38616077D-01  |
| KE0720 | 0.33808294D-04  |          |                 |                 | 293 411 0.30D-01 |
| KE0740 | I 22            | RPM2**** | 0.30238353D 02  | -0.75018223D 04 | -0.28252855D-01  |
| KE0740 | 0.18152509D-04  |          |                 |                 | 313 465 0.31D-01 |
| KE0800 | I 12            | RPM2**** | -0.58281733D 02 | 0.46022852D 04  | 0.19032262D 00   |
| KE0800 | -0.16244189D-03 |          |                 |                 | 293 447 0.13D 00 |
| KE0801 | I 11            | RPM2**** | -0.16377240D 02 | -0.14125767D 04 | 0.91139663D-01   |
| KE0801 | -0.82220634D-04 |          |                 |                 | 293 441 0.13D 00 |
| KE0802 | J 12            | RPM2**** | 0.51574275D 02  | -0.86523422D 04 | -0.10643159D 00  |
| KE0802 | 0.10186297D-03  |          |                 |                 | 288 424 0.19D 00 |
| KE0810 | I 11            | RPM2**** | 0.16856127D 02  | -0.52338853D 04 | -0.88892330D-04  |
| KE0810 | 0.75498105D-07  |          |                 |                 | 380 481 0.64D-03 |
| KE0830 | I 11            | RPM2**** | 0.16867186D 02  | -0.51189412D 04 | -0.88156709D-04  |
| KE0830 | 0.73679066D-07  |          |                 |                 | 359 461 0.45D-03 |
| KE0850 | I 8             | RPM2**** | 0.33729517D 02  | -0.82632914D 04 | -0.30963951D-01  |
| KE0850 | 0.22649922D-04  |          |                 |                 | 287 409 0.59D-01 |
| KE0870 | I 11            | RPM2**** | 0.17090378D 02  | -0.55896563D 04 | -0.45415371D-03  |
| KE0870 | 0.39330977D-06  |          |                 |                 | 279 381 0.21D-04 |

Table 10. Range 2 vapor pressure correlations--Continued

|        |   |                 |          |                 |                 |                  |
|--------|---|-----------------|----------|-----------------|-----------------|------------------|
| KE0890 | I | 13              | RPM2**** | 0.22435782D 02  | -0.67642090D 04 | -0.84645315D-02  |
| KE0890 |   | 0.20066396D-05  |          |                 |                 | 394 485 0.39D-01 |
| KE0910 | I | 4               | RIEDEL** | 0.23473348D 04  | -0.34498341D 03 | -0.11554548D 06  |
| KE0910 |   | 0.25357439D-14  |          |                 |                 | 332 457 0.76D-05 |
| KE0950 | G | 58              | VAPRES-2 | -0.26240368D 04 | 0.50707528D 05  | -0.13624744D 01  |
| KE0950 |   | 0.60820529D-03  |          | 0.49191888D 03  |                 | 303 476 0.16D 00 |
| KE0980 | J | 7               | RPM2**** | 0.63746621D 02  | -0.13829575D 05 | -0.95899972D-01  |
| KE0980 |   | 0.64946645D-04  |          |                 |                 | 415 511 0.42D-01 |
| KE1000 | I | 23              | VAPRES-2 | 0.25066182D 04  | -0.66711165D 05 | 0.11440382D 01   |
| KE1000 |   | -0.48792265D-03 |          | -0.45344764D 03 |                 | 333 469 0.35D-01 |
| KE1003 | C | 30              | WAGNER** | -0.86610867D 01 | 0.18792310D 01  | -0.54913237D 01  |
| KE1003 |   | -0.29722768D 01 |          | 0.64000000D 03  | 0.23199987D 01  | 298 480 0.74D-02 |
| KE1020 | I | 13              | VAPRES-2 | 0.40176615D 03  | -0.17039623D 05 | 0.12875484D 00   |
| KE1020 |   | -0.44344156D-04 |          | -0.66788250D 02 |                 | 333 454 0.10D-02 |
| KE1060 | I | 11              | RPM2**** | 0.17107479D 02  | -0.58037434D 04 | -0.41235569D-03  |
| KE1060 |   | 0.35515840D-06  |          |                 |                 | 299 401 0.34D-04 |
| KE1100 | I | 18              | RPM2**** | 0.42065341D 02  | -0.96075335D 04 | -0.56094570D-01  |
| KE1100 |   | 0.39838002D-04  |          |                 |                 | 333 494 0.73D-03 |
| KE1180 | I | 7               | RPM2**** | -0.31931183D 02 | 0.76175152D 03  | 0.11630691D 00   |
| KE1180 |   | -0.91697854D-04 |          |                 |                 | 405 491 0.56D-01 |
| KE1200 | I | 16              | RPM2**** | 0.18114459D 02  | -0.63943280D 04 | -0.20508118D-02  |
| KE1200 |   | 0.15259788D-05  |          |                 |                 | 369 511 0.70D-02 |
| KE1500 | I | 15              | RPM2**** | 0.44285192D 02  | -0.10504622D 05 | -0.57468922D-01  |
| KE1500 |   | 0.39224351D-04  |          |                 |                 | 353 424 0.20D-03 |
| KE1600 | I | 12              | RPM2**** | 0.16348405D 02  | -0.54532192D 04 | -0.13314052D-03  |
| KE1600 |   | 0.10961990D-06  |          |                 |                 | 369 481 0.17D-03 |
| KE1620 | H | 21              | RPM2**** | -0.73204088D 02 | 0.90466559D 04  | 0.18287068D 00   |
| KE1620 |   | -0.12508377D-03 |          |                 |                 | 451 500 0.33D 00 |
| KE1700 | I | 16              | RPM2**** | 0.17009724D 02  | -0.62063641D 04 | -0.10441452D-03  |
| KE1700 |   | 0.87991144D-07  |          |                 |                 | 369 521 0.32D-03 |
| KE1720 | I | 20              | RPM2**** | 0.99367506D 02  | -0.19759721D 05 | -0.17211686D 00  |
| KE1720 |   | 0.11966357D-03  |          |                 |                 | 375 535 0.44D-02 |
| KE1800 | K | 2               | RPM2**** | 0.15630510D 02  | -0.58530705D 04 | 0.00000000D 00   |
| KE1800 |   | 0.00000000D 00  |          |                 |                 | 395 403          |
| KE1820 | J | 11              | RPM2**** | 0.25265859D 02  | -0.47381032D 04 | -0.49092128D-01  |
| KE1820 |   | 0.47445496D-04  |          |                 |                 | 292 417 0.26D-01 |
| KE1821 | J | 8               | RPM2**** | -0.83424914D 02 | 0.52538877D 04  | 0.31324636D 00   |
| KE1821 |   | -0.33243093D-03 |          |                 |                 | 294 368 0.30D-01 |
| KE1900 | J | 5               | RPM2**** | -0.99897398D 02 | 0.12670804D 05  | 0.23088809D 00   |
| KE1900 |   | -0.14890088D-03 |          |                 |                 | 323 418 0.13D-01 |
| KE1901 | J | 8               | RPM2**** | 0.66819317D 04  | -0.92881114D 06 | -0.16059749D 02  |
| KE1901 |   | 0.12896429D-01  |          |                 |                 | 388 431 0.26D-01 |
| KE2100 | F | 33              | RPM2**** | 0.39858830D 02  | -0.10388870D 05 | -0.41013400D-01  |
| KE2100 |   | 0.23576007D-04  |          |                 |                 | 298 527 0.28D-01 |
| KE2104 | C | 30              | VAPRES-2 | 0.40188328D 03  | -0.19622726D 05 | 0.10659951D 00   |
| KE2104 |   | -0.31594792D-04 |          | -0.64916970D 02 |                 | 298 521 0.13D-01 |
| KE2120 | I | 7               | RPM2**** | -0.43389210D 02 | 0.30307622D 04  | 0.12861987D 00   |
| KE2120 |   | -0.92236652D-04 |          |                 |                 | 449 501 0.10D-01 |
| KE2225 | I | 22              | VAPRES-2 | -0.35752726D 03 | 0.13802298D 04  | -0.16995624D 00  |
| KE2225 |   | 0.63613684D-04  |          | 0.68760896D 02  |                 | 408 556 0.16D-01 |
| KE2261 | K | 2               | RPM2**** | 0.19418350D 02  | -0.84826264D 04 | 0.00000000D 00   |
| KE2261 |   | 0.00000000D 00  |          |                 |                 | 417 574          |

Table 10. Range 2 vapor pressure correlations--Continued

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE2300 | F 19            | VAPRES-2 | -0.62855974D 03 | 0.57720465D 04  | -0.31642310D 00  |
| KE2300 | 0.12610738D-03  |          | 0.12024952D 03  |                 | 333 542 0.53D-01 |
| KE2330 | J 10            | RPM2**** | 0.44650283D 02  | -0.11158370D 05 | -0.57059059D-01  |
| KE2330 | 0.40726555D-04  |          |                 |                 | 286 524 0.10D-01 |
| KE2331 | J 10            | RPM2**** | -0.19575553D 04 | 0.19631481D 06  | 0.63736451D 01   |
| KE2331 | -0.68379550D-02 |          |                 |                 | 291 330 0.25D-03 |
| KE2365 | G 41            | VAPRES-2 | -0.99581025D 03 | 0.18157724D 05  | -0.39969474D 00  |
| KE2365 | 0.13929486D-03  |          | 0.18137657D 03  |                 | 329 598 0.20D 00 |
| KE2460 | J 26            | RIEDEL** | 0.36652016D 03  | -0.48575010D 02 | -0.32112042D 05  |
| KE2460 | 0.28048558D-16  |          |                 |                 | 558 651 0.31D 00 |
| KE2473 | J 7             | RPM2**** | -0.22362756D 01 | -0.64738203D 04 | 0.43962829D-01   |
| KE2473 | -0.30566467D-04 |          |                 |                 | 474 724 0.38D-01 |
| KE2474 | J 22            | RPM2**** | 0.18832730D 03  | -0.38592193D 05 | -0.36089778D 00  |
| KE2474 | 0.26967276D-03  |          |                 |                 | 410 496 0.10D-02 |
| KE2477 | J 20            | RPM2**** | -0.35975370D 00 | -0.10541719D 05 | 0.76920902D-01   |
| KE2477 | -0.68264351D-04 |          |                 |                 | 373 457 0.51D-03 |
| KE2506 | C 14            | RPM2**** | 0.39391556D 02  | -0.11775235D 05 | -0.34494615D-01  |
| KE2506 | 0.17216390D-04  |          |                 |                 | 437 576 0.22D 00 |
| KE2545 | I 39            | RIEDEL** | 0.73424260D 02  | -0.76018739D 01 | -0.12094587D 05  |
| KE2545 | -0.21751014D-17 |          |                 |                 | 503 604 0.15D 00 |
| KE2775 | J 9             | RPM2**** | 0.54175963D 03  | -0.10033771D 06 | -0.10049879D 01  |
| KE2775 | 0.63820178D-03  |          |                 |                 | 456 549 0.12D-01 |
| KE3350 | K 2             | RPM2**** | 0.28106180D 02  | -0.14368583D 05 | 0.00000000D 00   |
| KE3350 | 0.00000000D 00  |          |                 |                 | 443 525          |

Table 11. Range 3 vapor pressure correlations

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE0300 | A 93            | WAGNER** | -0.76478446D 01 | 0.16786170D 01  | -0.32366434D 01  |
| KE0300 | -0.15276237D 01 |          | 0.50809985D 03  | 0.46999960D 01  | 247 398 0.96D-01 |
| KE0305 | I 12            | RPM2**** | 0.51708912D 02  | -0.74019867D 04 | -0.11732730D 00  |
| KE0305 | 0.12983094D-03  |          |                 |                 | 238 294 0.18D-01 |
| KE0360 | I 4             | RPM2**** | 0.63297187D 02  | -0.10289174D 05 | -0.13078063D 00  |
| KE0360 | 0.12264536D-03  |          |                 |                 | 303 392 0.46D-03 |
| KE0361 | I 4             | RPM2**** | 0.26169771D 02  | -0.55232119D 04 | -0.28809006D-01  |
| KE0361 | 0.24994206D-04  |          |                 |                 | 292 392 0.38D-03 |
| KE0362 | J 5             | RPM2**** | 0.43814304D 01  | -0.42660432D 04 | 0.37510628D-01   |
| KE0362 | -0.34712350D-04 |          |                 |                 | 348 446 0.33D-01 |
| KE0370 | I 11            | VAPRES-2 | 0.48887711D 03  | -0.12792830D 05 | 0.28424310D 00   |
| KE0370 | -0.15548657D-03 |          | -0.89800244D 02 |                 | 232 345 0.35D 00 |
| KE0380 | G 22            | WAGNER** | -0.74864472D 01 | 0.82054154D 00  | -0.29970338D 01  |
| KE0380 | -0.10487798D 02 |          | 0.35724463D 03  | 0.28411484D 01  | 194 304 0.12D 01 |
| KE0400 | A 49            | WAGNER** | -0.76396468D 01 | 0.15330646D 01  | -0.33071878D 01  |
| KE0400 | -0.22181141D 01 |          | 0.53677979D 03  | 0.42069960D 01  | 265 448 0.18D 00 |
| KE0410 | J 9             | RPM2**** | -0.36104822D 02 | 0.79123257D 03  | 0.17481982D 00   |
| KE0410 | -0.18881169D-03 |          |                 |                 | 260 363 0.33D 00 |
| KE0420 | H 16            | RPM2**** | 0.19664233D 02  | -0.49770013D 04 | -0.31815092D-02  |
| KE0420 | -0.34876835D-05 |          |                 |                 | 249 381 0.84D-01 |
| KE0430 | K 2             | RPM2**** | 0.16936190D 02  | -0.49228300D 04 | 0.00000000D 00   |
| KE0430 | 0.00000000D 00  |          |                 |                 | 343 400          |
| KE0440 | J 6             | RPM2**** | -0.25859342D 03 | 0.25691015D 05  | 0.84404370D 00   |
| KE0440 | -0.86319912D-03 |          |                 |                 | 300 355 0.64D 00 |
| KE0445 | J 13            | RPM2**** | -0.37836491D 03 | 0.46708999D 05  | 0.10059766D 01   |
| KE0445 | -0.85404877D-03 |          |                 |                 | 372 416 0.85D 00 |
| KE0446 | K 2             | RPM2**** | 0.17404000D 02  | -0.58193928D 04 | 0.00000000D 00   |
| KE0446 | 0.00000000D 00  |          |                 |                 | 343 456          |
| KE0450 | J 9             | RPM2**** | 0.68041358D 02  | -0.12469551D 05 | -0.12079499D 00  |
| KE0450 | 0.95103685D-04  |          |                 |                 | 322 428 0.80D-01 |
| KE0451 | J 8             | RPM2**** | 0.11101456D 03  | -0.16741801D 05 | -0.25145797D 00  |
| KE0451 | 0.22344785D-03  |          |                 |                 | 306 410 0.90D-01 |
| KE0460 | I 17            | RPM2**** | 0.16738657D 02  | -0.46777777D 04 | -0.33828305D-03  |
| KE0460 | 0.29316526D-06  |          |                 |                 | 309 391 0.18D-03 |
| KE0500 | E 27            | WAGNER** | -0.75098802D 01 | 0.98487982D 00  | -0.28407473D 01  |
| KE0500 | -0.41918431D 01 |          | 0.56107983D 03  | 0.36939983D 01  | 282 473 0.28D 00 |
| KE0501 | E 29            | WAGNER** | -0.64924142D 01 | -0.12998031D 01 | 0.20895716D 00   |
| KE0501 | -0.94551795D 01 |          | 0.56145996D 03  | 0.37289982D 01  | 282 473 0.12D 01 |
| KE0505 | B 25            | WAGNER** | -0.79425250D 01 | 0.20530981D 01  | -0.37421557D 01  |
| KE0505 | -0.34919809D 01 |          | 0.55339990D 03  | 0.38499985D 01  | 276 377 0.10D-01 |
| KE0510 | H 29            | RPM2**** | -0.48963358D 02 | 0.24378665D 04  | 0.19501662D 00   |
| KE0510 | -0.19254584D-03 |          |                 |                 | 289 412 0.17D 00 |
| KE0520 | I 28            | VAPRES-2 | 0.24376810D 03  | -0.11456854D 05 | 0.75261551D-01   |
| KE0520 | -0.24333219D-04 |          | -0.39526822D 02 |                 | 273 539 0.12D 01 |
| KE0530 | J 6             | RPM2**** | 0.16466401D 02  | -0.45368554D 04 | -0.35654411D-03  |
| KE0530 | 0.31524389D-06  |          |                 |                 | 355 380 0.00D 00 |
| KE0540 | J 5             | RPM2**** | -0.11112349D 03 | 0.10130898D 05  | 0.37424566D 00   |
| KE0540 | -0.36622482D-03 |          |                 |                 | 311 371 0.16D 00 |
| KE0555 | I 13            | RPM2**** | 0.17581976D 02  | -0.54557925D 04 | -0.54307219D-03  |
| KE0555 | 0.48989525D-06  |          |                 |                 | 272 333 0.11D-04 |
| KE0563 | I 5             | RPM2**** | -0.36593305D 02 | 0.11972196D 04  | 0.13428023D 00   |
| KEC563 | -0.10980973D-03 |          |                 |                 | 382 463 0.77D-02 |

Table 11. Range 3 vapor pressure correlations-Continued

|        |   |                 |          |                 |                 |                  |
|--------|---|-----------------|----------|-----------------|-----------------|------------------|
| KE0565 | I | 14              | RPM2**** | 0.20595620D 02  | -0.56476721D 04 | -0.66797188D-02  |
| KE0565 |   | 0.21173870D-05  |          |                 |                 | 317 419 0.18D 00 |
| KE0566 | I | 8               | RPM2**** | 0.41970324D 02  | -0.99808633D 04 | -0.52226934D-01  |
| KE0566 |   | 0.39833865D-04  |          |                 |                 | 317 459 0.85D-01 |
| KE0570 | I | 11              | RPM2**** | 0.31404936D 02  | -0.87815700D 04 | -0.32014182D-01  |
| KE0570 |   | 0.34129310D-04  |          |                 |                 | 277 333 0.13D-04 |
| KE0600 | C | 32              | WAGNER** | -0.81315482D 01 | 0.18766746D 01  | -0.42287461D 01  |
| KE0600 |   | -0.27338595D 01 |          | 0.58700000D 03  | 0.33229990D 01  | 298 428 0.38D-02 |
| KE0601 | C | 24              | WAGNER** | -0.79647906D 01 | 0.17198839D 01  | -0.42568912D 01  |
| KE0601 |   | -0.23051546D 01 |          | 0.58281982D 03  | 0.33199987D 01  | 298 407 0.35D-02 |
| KE0604 | H | 15              | WAGNER** | -0.69749525D 01 | -0.78241822D 00 | 0.41328603D 00   |
| KE0604 |   | -0.14350688D 02 |          | 0.57100000D 03  | 0.32699986D 01  | 283 484 0.13D 01 |
| KE0605 | J | 12              | RPM2**** | 0.67406874D 02  | -0.11369426D 05 | -0.12515635D 00  |
| KE0605 |   | 0.10012928D-03  |          |                 |                 | 300 389 0.52D 00 |
| KE0607 | C | 38              | WAGNER** | -0.76569055D 01 | 0.16102765D 01  | -0.36188184D 01  |
| KE0607 |   | -0.28748554D 01 |          | 0.56700000D 03  | 0.34699984D 01  | 284 406 0.71D-02 |
| KE0620 | H | 26              | WAGNER** | -0.86065609D 01 | 0.17456880D 01  | -0.13681218D 01  |
| KE0620 |   | -0.74119991D 01 |          | 0.62900000D 03  | 0.38499985D 01  | 302 533 0.12D 01 |
| KE0640 | I | 13              | RPM2**** | 0.12562638D 02  | -0.42869180D 04 | 0.11158413D-01   |
| KE0640 |   | -0.10948396D-04 |          |                 |                 | 401 561 0.15D 01 |
| KE0645 | I | 4               | RPM2**** | 0.41406877D 02  | -0.79886545D 04 | -0.61649738D-01  |
| KE0645 |   | 0.49977846D-04  |          |                 |                 | 273 395 0.49D-03 |
| KE0650 | J | 13              | RPM2**** | 0.40684782D 01  | -0.37767853D 04 | 0.45759886D-01   |
| KE0650 |   | -0.52451646D-04 |          |                 |                 | 287 404 0.13D 00 |
| KE0660 | J | 8               | RIEDEL** | 0.46007514D 04  | -0.67240180D 03 | -0.23440132D 06  |
| KE0660 |   | 0.41021702D-14  |          |                 |                 | 392 402 0.25D-01 |
| KE0670 | H | 15              | RPM2**** | 0.21864140D 02  | -0.64159922D 04 | -0.77320691D-02  |
| KE0670 |   | 0.36538030D-05  |          |                 |                 | 310 442 0.21D-02 |
| KE0680 | I | 4               | RPM2**** | -0.53089226D 02 | 0.31022259D 04  | 0.17381281D 00   |
| KE0680 |   | -0.14074304D-03 |          |                 |                 | 377 488 0.20D-02 |
| KE0700 | F | 46              | WAGNER** | -0.99483801D 01 | 0.47053877D 01  | -0.67889499D 01  |
| KE0700 |   | -0.17144393D 00 |          | 0.61150000D 03  | 0.34359989D 01  | 274 453 0.60D-01 |
| KE0702 | I | 7               | RPM2**** | 0.12619969D 02  | -0.44925265D 04 | 0.11623943D-01   |
| KE0702 |   | -0.11975873D-04 |          |                 |                 | 273 418 0.13D-01 |
| KE0710 | I | 11              | RPM2**** | 0.16894049D 02  | -0.49772008D 04 | -0.12070011D-03  |
| KE0710 |   | 0.99568801D-07  |          |                 |                 | 349 451 0.66D-03 |
| KE0720 | H | 15              | VAPRES-2 | 0.47099357D 03  | -0.15989232D 05 | 0.19827006D 00   |
| KE0720 |   | -0.79336319D-04 |          | -0.82270805D 02 |                 | 293 441 0.26D-01 |
| KE0740 | I | 22              | RPM2**** | 0.30238353D 02  | -0.75018223D 04 | -0.28252855D-01  |
| KE0740 |   | 0.18152509D-04  |          |                 |                 | 313 465 0.31D-01 |
| KE0800 | I | 12              | RPM2**** | -0.58281733D 02 | 0.46022852D 04  | 0.19032262D 00   |
| KE0800 |   | -0.16244189D-03 |          |                 |                 | 293 447 0.13D 00 |
| KE0801 | I | 11              | RPM2**** | -0.16377240D 02 | -0.14125767D 04 | 0.91139663D-01   |
| KE0801 |   | -0.82220634D-04 |          |                 |                 | 293 441 0.13D 00 |
| KE0802 | J | 12              | RPM2**** | 0.51574275D 02  | -0.86523422D 04 | -0.10643159D 00  |
| KE0802 |   | 0.10186297D-03  |          |                 |                 | 288 424 0.19D 00 |
| KE0810 | I | 11              | RPM2**** | 0.16856127D 02  | -0.52338853D 04 | -0.88892330D-04  |
| KE0810 |   | 0.75498105D-07  |          |                 |                 | 380 481 0.64D-03 |
| KE0830 | I | 11              | RPM2**** | 0.16867186D 02  | -0.51189412D 04 | -0.88156709D-04  |
| KE0830 |   | 0.73679066D-07  |          |                 |                 | 359 461 0.45D-03 |
| KE0850 | I | 8               | RPM2**** | 0.33729517D 02  | -0.82632914D 04 | -0.30963951D-01  |
| KE0850 |   | 0.22649922D-04  |          |                 |                 | 287 409 0.59D-01 |

Table 11. Range 3 vapor pressure correlations--Continued

|        |                 |           |                 |                 |                  |
|--------|-----------------|-----------|-----------------|-----------------|------------------|
| KE0870 | I 11            | RPM2***** | 0.17090378D 02  | -0.55896563D 04 | -0.45415371D-03  |
| KE0870 | 0.39330977D-06  |           |                 |                 | 279 381 0.21D-04 |
| KE0890 | I 13            | RPM2***** | 0.22435782D 02  | -0.67642090D 04 | -0.84645315D-02  |
| KE0890 | 0.20066396D-05  |           |                 |                 | 394 485 0.39D-01 |
| KE0910 | I 4             | RIEDEL**  | 0.23473348D 04  | -0.34498341D 03 | -0.11554548D 06  |
| KE0910 | 0.25357439D-14  |           |                 |                 | 332 457 0.76D-05 |
| KE0950 | G 58            | VAPRES-2  | -0.26240368D 04 | 0.50707528D 05  | -0.13624744D 01  |
| KE0950 | 0.60820529D-03  |           | 0.49191888D 03  |                 | 303 476 0.16D 00 |
| KE0980 | J 7             | RPM2***** | 0.63746621D 02  | -0.13829575D 05 | -0.95899972D-01  |
| KE0980 | 0.64946645D-04  |           |                 |                 | 415 511 0.42D-01 |
| KE1000 | I 23            | VAPRES-2  | 0.25066182D 04  | -0.66711165D 05 | 0.11440382D 01   |
| KE1000 | -0.48792265D-03 |           | -0.45344764D 03 |                 | 333 469 0.35D-01 |
| KE1003 | C 31            | WAGNER**  | -0.86650883D 01 | 0.18886549D 01  | -0.55050132D 01  |
| KE1003 | -0.29487241D 01 |           | 0.64000000D 03  | 0.23199987D 01  | 298 486 0.79D-02 |
| KE1020 | I 13            | VAPRES-2  | 0.40176615D 03  | -0.17039623D 05 | 0.12875484D 00   |
| KE1020 | -0.44344156D-04 |           | -0.66788250D 02 |                 | 333 454 0.10D-02 |
| KE1060 | I 11            | RPM2***** | 0.17107479D 02  | -0.58037434D 04 | -0.41235569D-03  |
| KE1060 | 0.35515840D-06  |           |                 |                 | 299 401 0.34D-04 |
| KE1100 | I 18            | RPM2***** | 0.42065341D 02  | -0.96075335D 04 | -0.56094570D-01  |
| KE1100 | 0.39838002D-04  |           |                 |                 | 333 494 0.73D-03 |
| KE1180 | I 7             | RPM2***** | -0.31931183D 02 | 0.76175152D 03  | 0.11630691D 00   |
| KE1180 | -0.91697854D-04 |           |                 |                 | 405 491 0.56D-01 |
| KE1200 | I 17            | RPM2***** | 0.17973910D 02  | -0.63745665D 04 | -0.17194104D-02  |
| KE1200 | 0.12669434D-05  |           |                 |                 | 369 521 0.85D-02 |
| KE1500 | I 15            | RPM2***** | 0.44285192D 02  | -0.10504622D 05 | -0.57468922D-01  |
| KE1500 | 0.39224351D-04  |           |                 |                 | 353 424 0.20D-03 |
| KE1600 | I 16            | RPM2***** | 0.16332197D 02  | -0.54509453D 04 | -0.94791231D-04  |
| KE1600 | 0.79497020D-07  |           |                 |                 | 369 521 0.66D-03 |
| KE1620 | H 21            | RPM2***** | -0.73204088D 02 | 0.90466559D 04  | 0.18287068D 00   |
| KE1620 | -0.12508377D-03 |           |                 |                 | 451 500 0.33D 00 |
| KE1700 | I 16            | RPM2***** | 0.17009724D 02  | -0.62063641D 04 | -0.10441452D-03  |
| KE1700 | 0.87991144D-07  |           |                 |                 | 369 521 0.32D-03 |
| KE1720 | I 20            | RPM2***** | 0.99367506D 02  | -0.19759721D 05 | -0.17211686D 00  |
| KE1720 | 0.11966357D-03  |           |                 |                 | 375 535 0.44D-02 |
| KE1800 | K 2             | RPM2***** | 0.15630510D 02  | -0.58530705D 04 | 0.00000000D 00   |
| KE1800 | 0.00000000D 00  |           |                 |                 | 395 403          |
| KE1820 | J 11            | RPM2***** | 0.25265859D 02  | -0.47381032D 04 | -0.49092128D-01  |
| KE1820 | 0.47445496D-04  |           |                 |                 | 292 417 0.26D-01 |
| KE1821 | J 8             | RPM2***** | -0.83424914D 02 | 0.52538877D 04  | 0.31324636D 00   |
| KE1821 | -0.33243093D-03 |           |                 |                 | 294 368 0.30D-01 |
| KE1900 | J 5             | RPM2***** | -0.99897398D 02 | 0.12670804D 05  | 0.23088809D 00   |
| KE1900 | -0.14890088D-03 |           |                 |                 | 323 418 0.13D-01 |
| KE1901 | J 8             | RPM2***** | 0.66819317D 04  | -0.92881114D 06 | -0.16059749D 02  |
| KE1901 | 0.12896429D-01  |           |                 |                 | 388 431 0.26D-01 |
| KE2100 | F 35            | RPM2***** | 0.39808738D 02  | -0.10382444D 05 | -0.40885275D-01  |
| KE2100 | 0.23468422D-04  |           |                 |                 | 298 539 0.36D-01 |
| KE2104 | C 32            | VAPRES-2  | 0.38789128D 03  | -0.19284923D 05 | 0.10027672D 00   |
| KE2104 | -0.29008985D-04 |           | -0.62369530D 02 |                 | 298 532 0.12D-01 |
| KE2120 | I 7             | RPM2***** | -0.43389210D 02 | 0.30307622D 04  | 0.12861987D 00   |
| KE2120 | -0.92236652D-04 |           |                 |                 | 449 501 0.10D-01 |
| KE2225 | I 23            | VAPRES-2  | -0.30334436D 03 | -0.12188523D 03 | -0.14965503D 00  |
| KE2225 | 0.56469159D-04  |           | 0.59179741D 02  |                 | 408 564 0.18D-01 |

Table 11. Range 3 vapor pressure correlations--Continued

|        |                 |          |                 |                 |                  |
|--------|-----------------|----------|-----------------|-----------------|------------------|
| KE2261 | K 2             | RPM2**** | 0.19418350D 02  | -0.84826264D 04 | 0.00000000D 00   |
| KE2261 | 0.00000000D 00  |          |                 |                 | 417 574          |
| KE2300 | F 19            | VAPRES-2 | -0.62855974D 03 | 0.57720465D 04  | -0.31642310D 00  |
| KE2300 | 0.12610738D-03  |          | 0.12024952D 03  |                 | 333 542 0.53D-01 |
| KE2330 | J 10            | RPM2**** | 0.44650283D 02  | -0.11158370D 05 | -0.57059059D-01  |
| KE2330 | 0.40726555D-04  |          |                 |                 | 286 524 0.10D-01 |
| KE2331 | J 10            | RPM2**** | -0.19575553D 04 | 0.19631481D 06  | 0.63736451D 01   |
| KE2331 | -0.68379550D-02 |          |                 |                 | 291 330 0.25D-03 |
| KE2365 | G 45            | VAPRES-2 | -0.73382832D 03 | 0.11307120D 05  | -0.29425735D 00  |
| KE2365 | 0.10027145D-03  |          | 0.13451238D 03  |                 | 329 622 0.30D 00 |
| KE2460 | J 26            | RIEDEL** | 0.36652016D 03  | -0.48575010D 02 | -0.32112042D 05  |
| KE2460 | 0.28048558D-16  |          |                 |                 | 558 651 0.31D 00 |
| KE2473 | J 7             | RPM2**** | -0.22362756D 01 | -0.64738203D 04 | 0.43962829D-01   |
| KE2473 | -0.30566467D-04 |          |                 |                 | 474 724 0.38D-01 |
| KE2474 | J 22            | RPM2**** | 0.18832730D 03  | -0.38592193D 05 | -0.36089778D 00  |
| KE2474 | 0.26967276D-03  |          |                 |                 | 410 496 0.10D-02 |
| KE2477 | J 20            | RPM2**** | -0.35975370D 00 | -0.10541719D 05 | 0.76920902D-01   |
| KE2477 | -0.68264351D-04 |          |                 |                 | 373 457 0.51D-03 |
| KE2506 | C 16            | RPM2**** | 0.50594333D 02  | -0.13634600D 05 | -0.56890913D-01  |
| KE2506 | 0.32071991D-04  |          |                 |                 | 437 601 0.51D 00 |
| KE2545 | I 39            | RIEDEL** | 0.73424260D 02  | -0.76018739D 01 | -0.12094587D 05  |
| KE2545 | -0.21751014D-17 |          |                 |                 | 503 604 0.15D 00 |
| KE2775 | J 9             | RPM2**** | 0.54175963D 03  | -0.10033771D 06 | -0.10049879D 01  |
| KE2775 | 0.63820178D-03  |          |                 |                 | 456 549 0.12D-01 |
| KE3350 | K 2             | RPM2**** | 0.28106180D 02  | -0.14368583D 05 | 0.00000000D 00   |
| KE3350 | 0.00000000D 00  |          |                 |                 | 443 525          |

Table 12. Range 4 vapor pressure correlations

|        |   |                 |          |                 |                 |                  |
|--------|---|-----------------|----------|-----------------|-----------------|------------------|
| KE0300 | A | 63              | WAGNER** | -0.74271578D 01 | 0.10922862D 01  | -0.19873034D 01  |
| KE0300 |   | -0.65774782D 01 |          | 0.50809985D 03  | 0.46999960D 01  | 309 509 0.12D 01 |
| KE0370 | I | 13              | RIEDEL** | 0.51987333D 02  | -0.54992005D 01 | -0.46055390D 04  |
| KE0370 |   | 0.59499181D-16  |          |                 |                 | 273 411 0.76D 00 |
| KE0380 | G | 29              | WAGNER** | -0.77804023D 01 | 0.17061565D 01  | -0.55119078D 01  |
| KE0380 |   | 0.36491593D 01  |          | 0.35724463D 03  | 0.28411484D 01  | 225 358 0.31D 01 |
| KE0400 | A | 49              | WAGNER** | -0.77821606D 01 | 0.19660930D 01  | -0.45547369D 01  |
| KE0400 |   | 0.51033664D 01  |          | 0.53677979D 03  | 0.42069960D 01  | 333 537 0.29D 01 |
| KE0420 | H | 5               | RPM2**** | -0.41338309D 02 | 0.26826805D 04  | 0.15847068D 00   |
| KE0420 |   | -0.14601138D-03 |          |                 |                 | 356 381 0.71D-02 |
| KE0500 | E | 30              | WAGNER** | -0.72551714D 01 | 0.25769821D 00  | -0.10269338D 01  |
| KE0500 |   | -0.12997027D 02 |          | 0.56107983D 03  | 0.36939983D 01  | 355 545 0.26D 01 |
| KE0501 | E | 31              | WAGNER** | -0.74645307D 01 | 0.15101506D 01  | -0.70957752D 01  |
| KE0501 |   | 0.29279142D 02  |          | 0.56145996D 03  | 0.37289982D 01  | 355 545 0.40D 01 |
| KE0505 | E | 25              | WAGNER** | -0.77016861D 01 | 0.20979165D 01  | -0.74639778D 01  |
| KE0505 |   | 0.32055908D 02  |          | 0.55339990D 03  | 0.38499985D 01  | 350 550 0.19D 01 |
| KE0510 | H | 6               | RIEDEL** | 0.33460813D 04  | -0.48757859D 03 | -0.17259015D 06  |
| KE0510 |   | 0.26929717D-14  |          |                 |                 | 393 412 0.30D-01 |
| KE0520 | I | 17              | VAPRES-2 | 0.37597781D 03  | -0.14596625D 05 | 0.13510762D 00   |
| KE0520 |   | -0.48500018D-04 |          | -0.63633082D 02 |                 | 388 539 0.16D 01 |
| KE0600 | C | 13              | WAGNER** | -0.82250937D 01 | 0.21242391D 01  | -0.47585480D 01  |
| KE0600 |   | -0.41166467D 00 |          | 0.58700000D 03  | 0.33229990D 01  | 385 428 0.32D-02 |
| KE0601 | C | 14              | WAGNER** | -0.77461734D 01 | 0.11668065D 01  | -0.32275202D 01  |
| KE0601 |   | -0.56463010D 01 |          | 0.58281982D 03  | 0.33199987D 01  | 379 407 0.20D-02 |
| KE0604 | I | 19              | WAGNER** | -0.77857409D 01 | 0.11556420D 01  | 0.14013432D 01   |
| KE0604 |   | -0.12915196D 03 |          | 0.57100000D 03  | 0.32699986D 01  | 388 567 0.16D 01 |
| KE0607 | C | 16              | WAGNER** | -0.76862355D 01 | 0.16766059D 01  | -0.36938294D 01  |
| KE0607 |   | -0.30089991D 01 |          | 0.56700000D 03  | 0.34699984D 01  | 362 406 0.87D-02 |
| KE0620 | J | 18              | WAGNER** | -0.77777529D 01 | -0.64181523D 00 | 0.44407638D 01   |
| KE0620 |   | -0.30293267D 02 |          | 0.62900000D 03  | 0.38499985D 01  | 413 582 0.59D 01 |
| KE0640 | I | 13              | RPM2**** | 0.12562638D 02  | -0.42869180D 04 | 0.11158413D-01   |
| KE0640 |   | -0.10948396D-04 |          |                 |                 | 401 561 0.15D 01 |
| KE0700 | C | 11              | WAGNER** | -0.11049744D 02 | 0.76039453D 01  | -0.12885185D 02  |
| KE0700 |   | 0.25715023D 02  |          | 0.61150000D 03  | 0.34359989D 01  | 407 453 0.12D-01 |
| KE0710 | I | 7               | RPM2**** | 0.16781712D 02  | -0.49615208D 04 | 0.14711739D-03   |
| KE0710 |   | -0.11291159D-06 |          |                 |                 | 390 451 0.71D-03 |
| KE0720 | H | 7               | RIEDEL** | 0.16486399D 02  | -0.20851789D-01 | -0.46599068D 04  |
| KE0720 |   | 0.11864683D-18  |          |                 |                 | 380 441 0.40D-03 |
| KE0740 | I | 7               | RPM2**** | 0.43399170D 01  | -0.36523985D 04 | 0.29850045D-01   |
| KE0740 |   | -0.25314379D-04 |          |                 |                 | 433 465 0.14D-01 |
| KE0950 | G | 5               | RPM2**** | 0.11470231D 02  | -0.50556512D 04 | 0.13641999D-01   |
| KE0950 |   | -0.11936343D-04 |          |                 |                 | 458 476 0.00D 00 |
| KE1003 | C | 11              | WAGNER** | -0.84860074D 01 | 0.13629362D 01  | -0.40025845D 01  |
| KE1003 |   | -0.13687968D 02 |          | 0.64000000D 03  | 0.23199987D 01  | 443 486 0.41D-02 |
| KE1020 | I | 4               | RPM2**** | 0.29270221D 02  | -0.73333600D 04 | -0.24539657D-01  |
| KE1020 |   | 0.14337444D-04  |          |                 |                 | 423 454 0.59D-03 |
| KE1200 | I | 5               | RPM2**** | 0.17958869D 02  | -0.63834928D 04 | -0.15442724D-02  |
| KE1200 |   | 0.10486322D-05  |          |                 |                 | 480 521 0.21D-03 |
| KE1600 | I | 8               | RPM2**** | 0.16259752D 02  | -0.54395626D 04 | 0.58457462D-04   |
| KE1600 |   | -0.28264046D-07 |          |                 |                 | 450 521 0.11D-02 |
| KE1620 | H | 12              | RPM2**** | 0.67655826D 03  | -0.11139630D 06 | -0.13723823D 01  |
| KE1620 |   | 0.94992874D-03  |          |                 |                 | 464 500 0.35D 00 |

Table 12. Range 4 vapor pressure correlations--Continued

|        |   |    |                 |                 |                 |                 |
|--------|---|----|-----------------|-----------------|-----------------|-----------------|
| KE1700 | I | 4  | RPM2****        | 0.18340928D 02  | -0.64288041D 04 | -0.27587607D-02 |
| KE1700 |   |    | 0.18513966D-05  |                 | 490             | 521 0.15D-03    |
| KE2100 | C | 10 | RPM2****        | 0.57404325D 02  | -0.13487763D 05 | -0.74065949D-01 |
| KE2100 |   |    | 0.44291422D-04  |                 | 493             | 539 0.22D-01    |
| KE2104 | C | 11 | RPM2****        | 0.33956207D 02  | -0.92916871D 04 | -0.29565440D-01 |
| KE2104 |   |    | 0.16060508D-04  |                 | 481             | 532 0.14D-01    |
| KE2225 | I | 6  | RPM2****        | 0.12036858D 02  | -0.58199290D 04 | 0.10284643D-01  |
| KE2225 |   |    | -0.82201750D-05 |                 | 520             | 564 0.24D-01    |
| KE2365 | G | 26 | VAPRES-2        | 0.16527152D 05  | -0.57617584D 06 | 0.45684349D 01  |
| KE2365 |   |    | -0.12489337D-02 | -0.27909133D 04 | 560             | 622 0.19D 00    |
| KE2460 | J | 7  | RIEDEL**        | 0.17529189D 05  | -0.24029397D 04 | -0.13170764D 07 |
| KE2460 |   |    | 0.86815023D-15  |                 | 630             | 651 0.18D 00    |
| KE2506 | C | 6  | RPM2****        | 0.42746661D 03  | -0.84065918D 05 | -0.72805420D 00 |
| KE2506 |   |    | 0.42989476D-03  |                 | 562             | 601 0.17D 00    |

### 5.2.1. Quality Ratings for Correlations

The quality rating symbols are defined in Table 13. Note that ratings A through F all involve experimental data from a "reliable source". A reliable source is one which has reported high-quality data for a large number of compounds and those data consistently agree with other good data. Only one source met these criteria for the ketone vapor pressure data--the National Physical Laboratory, Teddington, Middlesex, U. K. Very good vapor pressure data have been reported for the ketones by Collerson et al. [4418], Ambrose et al. [10253], and Ambrose et al. [10318] and, whenever a data set from one of those papers is involved, one of the A through F ratings will appear. For ratings A through C, the data from the reliable source cover the entire correlation range and the amount of corroboration from other sources ranges from substantial for A through partial for B to none for C. For ratings D through F, the reliable source data set covers only part of the correlation range and the three ratings differ only in the amount of corroborating data.

Ratings G through K do not involve a reliable source data set. A G rating tells the user that at least two data sets from different sources showed considerable agreement, whereas an H rating says that all the sources showed substantial disagreement. Both the G and H ratings indicate a better situation than the I and J ratings which indicate that only one source of data was available in any given temperature range.

Table 13. Definition of quality rating symbols  
for the individual property correlations

| Rating | Definition   |
|--------|--|
| A      | Correlation is based on extensive experimental data from a reliable source, and those data are substantiated by measurements from other sources over all or most of the range.   |
| B      | Correlation is based on extensive experimental data from a reliable source, but those data are substantiated by measurements from other sources over only part of the range.   |
| C      | Correlation is based on extensive experimental data from a reliable source, but the correlation is not corroborated by other measurements in any major part of the range.  |
| D      | Correlation is based on extensive experimental data from a reliable source over a major part of the range and on a less reliable data set in the other part. Data from other sources support the general validity of the correlation in both parts of the range.   |
| E      | Correlation is based on extensive experimental data from a reliable source over a major part of the range and on a less reliable data set in the other part. Data from other sources corroborate the data from the reliable source but supporting data are not available for the less reliable data set. |
| F      | Correlation is based on extensive experimental data from a reliable source over a major part of the range and on a less reliable data set in the other part. Neither part of the correlation is corroborated by measurements from other sources.   |
| G      | Correlation is based on data from two or more overlapping sources which through their mutual agreement support the validity of the correlation through an important part of its range.   |
| H      | Correlation is based on a group of points from a single source or from multiple sources which has been selected from among various disagreeing data sets or scattered data points from several sources.  |

Table 13. Definition of quality rating symbols  
for the individual property correlations--Continued

- 
- I Correlation is based on relatively smooth multiple data points from one source, or from two or more sources which do not overlap much, and there is little or no data available from other sources.
  - J Correlation is based on scattered data points from one or two sources.
  - K Correlation is just a straight line fit of only two or more data points from one or more sources.

The K rating indicates the correlation is just a straight-line fit of two or three data points. The only justification for including such correlations is the desire to provide the user with as much information as possible. Two elementary precautions were taken. First, the points fitted were usually required to be from the same source; points from different sources were used only if there were other corroborating measurements which supported the general accuracy of the two or three points fitted to the straight line. Second, the slope of the linear fit was checked to make sure it had the right sign and a reasonable numerical value. The possible pitfalls in the use of such a correlation are obvious and users are warned to be cautious in their use of property values obtained from such correlations.

In general, the quality of the experimental data base decreases as one goes from A to K in Table 13, but there can be exceptions to that rule. For example, for the D through F quality ratings, only part of the correlation is supported by a reliable source data set and it is possible for the other part to be less accurate than another correlation given a G rating. Another example concerns the I rating which presumably is superior to the J rating because the I data points are smooth whereas the J data are scattered. However, the I data may be smooth because it was reported only in equation form; it may be that the original raw data which the reporting authors smoothed were more scattered than other data sets which were given a J rating.

It is not possible to characterize precisely all the experimental circumstances which can arise with a limited number of single-character quality rating symbols, and the user may feel that the definition of the assigned rating may be imprecise in some instances. That is inevitable with only eleven symbols, but the addition of more soon becomes self-defeating. Also, the user must remember that the assigned symbol describes the total experimental data base originally available before the deletions began, and not just the final selected points which were actually correlated.

#### 5.2.2. Vapor Pressure Correlations

Following the quality rating symbol in the first line for each compound in tables 9, 10, 11 and 12 is another item related to the quality of the correlation data base--the number of selected experimental points fitted. In general, the larger the number of points the better.

The equation used for each compound-range combination is indicated by an eight character identifier. The identifier which appears in the first line for each compound is easily related to the corresponding vapor pressure equation in table 2. The other three items following the identifier in the first line are the first three constants (A, B, C) in the correlation equation. The D constant and the E constant (Vapres-2 equation only) appear on the second line. Only the Wagner equation has six constants--the  $T_c$  and  $P_c$  values used in the correlation are listed after the A,B,C,D constants. The  $T_c$  and  $P_c$  units are kelvin and megapascals, and in this report the values listed in tables 9 through 12 will always be the same as those listed in table 7. As a matter of policy, any compound constant values which are used in any correlation are always stored in the data bank with the correlation constants--in addition to storage in the compound constants section--so that the correlation can continue to be used even if the compound constant values stored in the compound constant section are changed.

The last three items at the end of the second line are the lower temperature limit, the higher temperature limit, and the root-mean-squared-deviation (rmsd) value for the fit. The lower temperature limit is the temperature of the lowest-temperature selected data point covered by the correlation rounded down to the next integer value. The higher limit is the temperature of the highest-temperature point rounded up to the next whole number. The actual range of any specific correlation is given by these lower and upper temperature limits and not by the nominal limits for that particular temperature range defined in section 4.2.3.

The rmsd value is in kilopascals and will range from a relatively low number for the range 2 fit to a higher number for the range 4 fit, the difference being due to the different magnitudes of the data points being fitted. The large variation in the magnitude of the vapor pressure data values with temperature makes it difficult to determine the significance of a given rmsd value. One should compare rmsd values only between fits for the same temperature range but even then the comparison may be meaningless. For example, the rmsd value for a range 4 fit where the selected data points cover the entire nominal temperature range from ( $T_b - 20$ ) to  $T_c$  will be very different from the rmsd for another range 4 fit where the data points are limited to the range from ( $T_b - 20$ ) to  $T_b$ . In any case, the rmsd is an indicator primarily of the amount of scatter in the data points fitted. If the data points being fitted are the raw (unsmoothed) data points measured by the authors, a low rmsd value can be considered to be an indicator of quality. However, a very low rmsd may not be significant--it may mean that the only available experimental data were reported in equation form and hence smoothed values had to be correlated.

In a superficial judging of the quality of a correlation, the user should rely primarily on the quality rating symbol as defined in table 13. The number of points available for fitting should be considered second and the rmsd value third.

### 5.3. Liquid Density

Tables 14, 15, 16 and 17 contain the constants for the liquid density correlations for ranges 1, 2, 3 and 4. The organization of the tables is the same as for the vapor pressure tables (tables 9, 10, 11 and 12), with two lines per correlation. The compound identification begins both lines. The quality rating (second item on the first line) has the same significance as for the vapor pressure and is defined by Table 13. The number of experimental points actually fitted by the correlation follows the quality rating.

The equation identifier (fourth item in the first line for each compound) is related to the equations in table 3. The low-range Francis equation (identifier is FRANCIS1) has four constants, A, B, C and E; the fourth constant is E rather than D in order to avoid confusion with the symbol for the density. The  $T_c$  value (if one is available) is also stored with the low range equation. The  $T_c$  is used only in defining the fitting ranges but the  $(T_c - 10)$  value used for the upper limit of the range 1 and range 4 fits with program FRANCIS1 can change enough with the  $T_c$  value to include or exclude a data point in a region where data points are sparse and thus have a relatively strong influence on the fitting process.

The high range Francis equation (identifier is FRANCIS2) sometimes used for range 4 has two adjustable constants A and B followed by the  $d_c$  and  $T_c$  values. The latter two appear in the equation and are listed here so that an old correlation will still be useable even if the values of  $V_c$  and  $T_c$  stored in the compound constants part of the data bank are changed.

Table 14. Range 1 liquid density correlations

|        |                |          |                |                |                    |
|--------|----------------|----------|----------------|----------------|--------------------|
| KE0300 | D 58           | FRANCIS1 | 0.11210213D 01 | 0.10215563D-02 | 0.79379501D 01     |
| KE0300 | 0.53905884D 03 |          | 0.50809985D 03 |                | 178 498 0.95D-03   |
| KE0340 | K 3            | FRANCIS1 | 0.13919132D 01 | 0.10882850D-02 | 0.00000000D 00     |
| KE0340 | 0.00000000D 00 |          |                |                | 277 299            |
| KE0380 | H 12           | FRANCIS1 | 0.23480034D 01 | 0.25871226D-02 | 0.31269958D 02     |
| KE0380 | 0.42212915D 03 |          | 0.35713477D 03 |                | 210 295 0.14D-02   |
| KE0400 | G 47           | FRANCIS1 | 0.11104259D 01 | 0.81403158D-03 | 0.19753296D 02     |
| KE0400 | 0.58889380D 03 |          | 0.53677979D 03 |                | 195 324 0.17D-03   |
| KE0420 | I 13           | FRANCIS1 | 0.12236357D 01 | 0.87728817D-03 | 0.74975948D 01     |
| KE0420 | 0.52308423D 03 |          |                |                | 273 363 0.51D-03   |
| KE0430 | I 9            | FRANCIS1 | 0.14537134D 01 | 0.10908672D-02 | 0.14505398D 02     |
| KE0430 | 0.65764941D 03 |          |                |                | 282 303 0.14D-03   |
| KE0500 | H 9            | FRANCIS1 | 0.10936251D 01 | 0.96370699D-03 | 0.48774409D 00     |
| KE0500 | 0.42092505D 03 |          | 0.56107983D 03 |                | 233 354 0.11D-03   |
| KE0501 | H 19           | FRANCIS1 | 0.10943232D 01 | 0.86304802D-03 | 0.70360441D 01     |
| KE0501 | 0.55340259D 03 |          | 0.56145996D 03 |                | 273 348 0.66D-04   |
| KE0505 | K 3            | FRANCIS1 | 0.10588190D 01 | 0.84827400D-03 | 0.00000000D 00     |
| KE0505 | 0.00000000D 00 |          |                |                | 283 324            |
| KE0510 | H 27           | FRANCIS1 | 0.12644968D 01 | 0.89787156D-03 | 0.80934544D 01     |
| KE0510 | 0.61981030D 03 |          |                |                | 277 374 0.20D-03   |
| KE0520 | H 15           | FRANCIS1 | 0.12307463D 01 | 0.95416536D-03 | 0.36097822D 01     |
| KE0520 | 0.17891855D 04 |          |                |                | 273 364 0.12D-03   |
| KE0530 | I 4            | FRANCIS1 | 0.11695671D 01 | 0.90240128D-03 | 0.82282317D 00     |
| KE0530 | 0.43741748D 03 |          |                |                | 293 . 361 0.59D-04 |
| KE0540 | K 3            | FRANCIS1 | 0.11309113D 01 | 0.95017100D-03 | 0.00000000D 00     |
| KE0540 | 0.00000000D 00 |          |                |                | 293 299            |
| KE0563 | K 2            | FRANCIS1 | 0.12291625D 01 | 0.82216200D-03 | 0.00000000D 00     |
| KE0563 | 0.00000000D 00 |          |                |                | 293 299            |
| KE0568 | K 2            | FRANCIS1 | 0.14145337D 01 | 0.11002640D-02 | 0.00000000D 00     |
| KE0568 | 0.00000000D 00 |          |                |                | 293 299            |
| KE0600 | H 7            | FRANCIS1 | 0.10629501D 01 | 0.76617324D-03 | 0.67085629D 01     |
| KE0600 | 0.54074902D 03 |          | 0.58700000D 03 |                | 283 334 0.18D-03   |
| KE0601 | I 4            | FRANCIS1 | 0.10622683D 01 | 0.75031724D-03 | 0.48805723D 01     |
| KE0601 | 0.47581445D 03 |          | 0.58281982D 03 |                | 297 324 0.14D-04   |
| KE0604 | H 18           | FRANCIS1 | 0.10666428D 01 | 0.82335575D-03 | 0.69826603D 01     |
| KE0604 | 0.57530029D 03 |          | 0.57100000D 03 |                | 273 374 0.11D-03   |
| KE0607 | I 13           | FRANCIS1 | 0.10912037D 01 | 0.94584492D-03 | 0.63908215D 01     |
| KE0607 | 0.12265347D 04 |          | 0.56700000D 03 |                | 293 354 0.29D-04   |
| KE0610 | K 2            | FRANCIS1 | 0.11699327D 01 | 0.67871500D-03 | 0.00000000D 00     |
| KE0610 | 0.00000000D 00 |          |                |                | 293 299            |
| KE0615 | J 21           | FRANCIS1 | 0.12592354D 01 | 0.73114224D-03 | 0.24115524D 02     |
| KE0615 | 0.65499878D 03 |          |                |                | 277 374 0.51D-03   |
| KE0620 | H 15           | FRANCIS1 | 0.12110815D 01 | 0.84087066D-03 | 0.62623587D 01     |
| KE0620 | 0.64040259D 03 |          | 0.62900000D 03 |                | 273 354 0.49D-04   |
| KE0625 | K 3            | FRANCIS1 | 0.11754525D 01 | 0.89549800D-03 | 0.00000000D 00     |
| KE0625 | 0.00000000D 00 |          |                |                | 293 361            |
| KE0650 | I 6            | FRANCIS1 | 0.11541748D 01 | 0.92861406D-03 | 0.12769001D 02     |
| KE0650 | 0.83510986D 03 |          |                |                | 293 394 0.43D-04   |
| KE0660 | I 4            | FRANCIS1 | 0.15105515D 01 | 0.97980653D-03 | 0.19811020D 02     |
| KE0660 | 0.90835181D 03 |          |                |                | 395 434 0.17D-03   |
| KE0670 | I 6            | FRANCIS1 | 0.12066355D 01 | 0.88522420D-03 | 0.25476007D 01     |
| KE0670 | 0.59638232D 03 |          |                |                | 293 394 0.18D-03   |

Table 14. Range 1 liquid density correlations--Continued

|        |                |          |                |                |                  |
|--------|----------------|----------|----------------|----------------|------------------|
| KE0700 | G 16           | FRANCIS1 | 0.10823164D 01 | 0.68128319D-03 | 0.28077332D 02   |
| KE0700 | 0.71180640D 03 |          | 0.61150000D 03 |                | 288 429 0.10D-03 |
| KE0701 | I 7            | FRANCIS1 | 0.10566082D 01 | 0.76659396D-03 | 0.29826403D 01   |
| KE0701 | 0.51027295D 03 |          |                |                | 288 360 0.14D-03 |
| KE0702 | H 10           | FRANCIS1 | 0.10744505D 01 | 0.73973392D-03 | 0.12342205D 02   |
| KE0702 | 0.59130103D 03 |          |                |                | 253 394 0.41D-03 |
| KE0720 | G 24           | FRANCIS1 | 0.10650043D 01 | 0.79409732D-03 | 0.79816027D 01   |
| KE0720 | 0.59359106D 03 |          |                |                | 283 374 0.39D-03 |
| KE0725 | I 20           | FRANCIS1 | 0.12179537D 01 | 0.80069271D-03 | 0.10817964D 02   |
| KE0725 | 0.63199292D 03 |          |                |                | 288 374 0.18D-03 |
| KE0730 | I 18           | FRANCIS1 | 0.12222862D 01 | 0.81374589D-03 | 0.84028273D 01   |
| KE0730 | 0.60423389D 03 |          |                |                | 277 374 0.10D-03 |
| KE0735 | I 13           | FRANCIS1 | 0.13543797D 01 | 0.89812255D-03 | 0.94656706D 01   |
| KE0735 | 0.10463357D 04 |          |                |                | 313 374 0.31D-03 |
| KE0740 | I 7            | FRANCIS1 | 0.11986494D 01 | 0.81006484D-03 | 0.38449039D 01   |
| KE0740 | 0.65876953D 03 |          |                |                | 297 374 0.75D-04 |
| KE0745 | J 7            | FRANCIS1 | 0.11601934D 01 | 0.70832646D-03 | 0.10340004D 02   |
| KE0745 | 0.66066748D 03 |          |                |                | 292 357 0.14D-02 |
| KE0746 | J 6            | FRANCIS1 | 0.11473150D 01 | 0.77219424D-03 | 0.26848648D 02   |
| KE0746 | 0.44958086D 04 |          |                |                | 291 361 0.78D-03 |
| KE0747 | G 8            | FRANCIS1 | 0.11351528D 01 | 0.70543634D-03 | 0.90721703D 00   |
| KE0747 | 0.37699731D 03 |          |                |                | 291 360 0.37D-02 |
| KE0760 | I 5            | FRANCIS1 | 0.13968458D 01 | 0.88775204D-03 | 0.16219463D 01   |
| KE0760 | 0.61806470D 03 |          |                |                | 348 401 0.42D-03 |
| KE0800 | H 17           | FRANCIS1 | 0.10774565D 01 | 0.79408265D-03 | 0.89678802D 01   |
| KE0800 | 0.64906519D 03 |          |                |                | 253 434 0.26D-03 |
| KE0801 | I 6            | FRANCIS1 | 0.10447025D 01 | 0.75790938D-03 | 0.56298885D-01   |
| KE0801 | 0.37720679D 03 |          |                |                | 293 360 0.13D-03 |
| KE0802 | K 3            | FRANCIS1 | 0.10581158D 01 | 0.81718800D-03 | 0.00000000D 00   |
| KE0802 | 0.00000000D 00 |          |                |                | 297 324          |
| KE0850 | K 2            | FRANCIS1 | 0.10557714D 01 | 0.85020700D-03 | 0.00000000D 00   |
| KE0850 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0890 | I 8            | FRANCIS1 | 0.11752396D 01 | 0.74465154D-03 | 0.23469505D 01   |
| KE0890 | 0.55955298D 03 |          |                |                | 329 412 0.72D-04 |
| KE0910 | K 3            | FRANCIS1 | 0.11457132D 01 | 0.83233000D-03 | 0.00000000D 00   |
| KE0910 | 0.00000000D 00 |          |                |                | 273 294          |
| KE0930 | I 20           | FRANCIS1 | 0.12116728D 01 | 0.71956799D-03 | 0.64043417D 01   |
| KE0930 | 0.51158325D 03 |          |                |                | 277 374 0.13D-03 |
| KE0950 | H 17           | FRANCIS1 | 0.12849731D 01 | 0.82102115D-03 | 0.73394318D 01   |
| KE0950 | 0.74487476D 03 |          |                |                | 293 475 0.84D-04 |
| KE0980 | K 2            | FRANCIS1 | 0.14689927D 01 | 0.94420500D-03 | 0.00000000D 00   |
| KE0980 | 0.00000000D 00 |          |                |                | 293 299          |
| KE1000 | H 16           | FRANCIS1 | 0.10667076D 01 | 0.69098081D-03 | 0.18308731D 02   |
| KE1000 | 0.71997681D 03 |          |                |                | 298 439 0.74D-04 |
| KE1001 | J 4            | FRANCIS1 | 0.10525827D 01 | 0.76424866D-03 | 0.19214630D 02   |
| KE1001 | 0.30584688D 04 |          |                |                | 293 359 0.25D-02 |
| KE1002 | K 3            | FRANCIS1 | 0.10635706D 01 | 0.82080900D-03 | 0.00000000D 00   |
| KE1002 | 0.00000000D 00 |          |                |                | 297 324          |
| KE1003 | H 8            | FRANCIS1 | 0.10534096D 01 | 0.79098716D-03 | 0.49999952D-02   |
| KE1003 | 0.88935620D 03 |          | 0.64000000D 03 |                | 283 360 0.49D-03 |
| KE1020 | I 6            | FRANCIS1 | 0.10386066D 01 | 0.75689703D-03 | 0.34747953D 01   |
| KE1020 | 0.60697998D 03 |          |                |                | 293 359 0.22D-03 |

Table 14. Range 1 liquid density correlations--Continued

|        |                |                |                 |                  |
|--------|----------------|----------------|-----------------|------------------|
| KE1040 | K 2 FRANCIS1   | 0.10481059D 01 | 0.76418900D-03  | 0.00000000D 00   |
| KE1040 | 0.00000000D 00 |                |                 | 293 299          |
| KE1150 | I 4 FRANCIS1   | 0.11017246D 01 | 0.64413319D-03  | 0.50127020D 01   |
| KE1150 | 0.49241553D 03 |                |                 | 303 363 0.56D-05 |
| KE1180 | I 4 FRANCIS1   | 0.12283163D 01 | 0.72272122D-03  | 0.87706625D 00   |
| KE1180 | 0.43193555D 03 |                |                 | 293 359 0.10D-03 |
| KE1181 | I 7 FRANCIS1   | 0.12354736D 01 | 0.75112213D-03  | 0.29371872D 01   |
| KE1181 | 0.51115088D 03 |                |                 | 293 359 0.28D-03 |
| KE1250 | I 9 FRANCIS1   | 0.13698235D 01 | 0.83868415D-03  | 0.96535120D 01   |
| KE1250 | 0.10811353D 04 |                |                 | 313 354 0.22D-03 |
| KE1320 | K 2 FRANCIS1   | 0.11775263D 01 | 0.82878800D-03  | 0.00000000D 00   |
| KE1320 | 0.00000000D 00 |                |                 | 289 294          |
| KE1350 | K 3 FRANCIS1   | 0.19414714D 01 | 0.12592340D-02  | 0.00000000D 00   |
| KE1350 | 0.00000000D 00 |                |                 | 306 347          |
| KE1360 | K 3 FRANCIS1   | 0.14523771D 01 | 0.95708700D-03  | 0.00000000D 00   |
| KE1360 | 0.00000000D 00 |                |                 | 292 362          |
| KE1400 | K 3 FRANCIS1   | 0.10606149D 01 | 0.80690800D-03  | 0.00000000D 00   |
| KE1400 | 0.00000000D 00 |                |                 | 288 304          |
| KE1401 | I 4 FRANCIS1   | 0.10355082D 01 | 0.68153860D-03  | 0.24201708D 01   |
| KE1401 | 0.52146802D 03 |                |                 | 293 359 0.71D-04 |
| KE1403 | K 3 FRANCIS1   | 0.10556330D 01 | 0.78969400D-03  | 0.00000000D 00   |
| KE1403 | 0.00000000D 00 |                |                 | 297 324          |
| KE1530 | I 7 FRANCIS1   | 0.11216106D 01 | 0.75179804D-03  | 0.11565094D 01   |
| KE1530 | 0.58048584D 03 |                |                 | 273 374 0.47D-04 |
| KE1550 | I 5 FRANCIS1   | 0.11585274D 01 | 0.88412291D-03  | 0.99014626D 01   |
| KE1550 | 0.11632017D 04 |                |                 | 287 294 0.14D-04 |
| KE1580 | J 6 FRANCIS1   | 0.11929045D 01 | 0.71501243D-03  | 0.31916519D 02   |
| KE1580 | 0.73905195D 04 |                |                 | 291 359 0.76D-03 |
| KE1620 | K 3 FRANCIS1   | 0.12227294D 01 | 0.85964500D-03  | 0.00000000D 00   |
| KE1620 | 0.00000000D 00 |                |                 | 453 474          |
| KE1640 | K 3 FRANCIS1   | 0.11054682D 01 | 0.64550500D-03  | 0.00000000D 00   |
| KE1640 | 0.00000000D 00 |                |                 | 286 294          |
| KE1660 | K 2 FRANCIS1   | 0.12286730D 01 | 0.10305550D-02  | 0.00000000D 00   |
| KE1660 | 0.00000000D 00 |                |                 | 289 294          |
| KE1680 | K 2 FRANCIS1   | 0.12271983D 01 | 0.10002810D-02  | 0.00000000D 00   |
| KE1680 | 0.00000000D 00 |                |                 | 288 294          |
| KE1750 | I 7 FRANCIS1   | 0.11910629D 01 | 0.65790350D-03  | 0.14866219D 01   |
| KE1750 | 0.44262402D 03 |                |                 | 291 360 0.26D-03 |
| KE1760 | I 4 FRANCIS1   | 0.12143669D 01 | 0.771111414D-03 | 0.56137331D-01   |
| KE1760 | 0.37699731D 03 |                |                 | 293 360 0.21D-04 |
| KE1762 | I 4 FRANCIS1   | 0.11962500D 01 | 0.70684613D-03  | 0.24943739D 00   |
| KE1762 | 0.39578760D 03 |                |                 | 298 361 0.45D-06 |
| KE1860 | I 8 FRANCIS1   | 0.13859816D 01 | 0.94468961D-03  | 0.49999952D-02   |
| KE1860 | 0.49347217D 03 |                |                 | 333 374 0.92D-03 |
| KE2000 | I 4 FRANCIS1   | 0.16353292D 01 | 0.10515784D-02  | 0.53056593D 01   |
| KE2000 | 0.85100244D 03 |                |                 | 296 354 0.18D-03 |
| KE2100 | G 28 FRANCIS1  | 0.10617561D 01 | 0.66399807D-03  | 0.19551086D 02   |
| KE2100 | 0.76776074D 03 |                |                 | 293 434 0.88D-04 |
| KE2104 | I 5 FRANCIS1   | 0.10162287D 01 | 0.57980116D-03  | 0.45092754D 01   |
| KE2104 | 0.50070825D 03 |                |                 | 293 360 0.12D-03 |
| KE2120 | I 9 FRANCIS1   | 0.11690245D 01 | 0.72760601D-03  | 0.35297394D 01   |
| KE2120 | 0.16314060D 04 |                |                 | 301 412 0.11D-03 |

Table 14. Range 1 liquid density correlations--Continued

|        |   |                |          |                |                |                |
|--------|---|----------------|----------|----------------|----------------|----------------|
| KE2130 | I | 4              | FRANCIS1 | 0.12822104D 01 | 0.88562258D-03 | 0.85805788D 01 |
| KE2130 |   | 0.38810552D 04 |          |                | 289 352        | 0.20D-03       |
| KE2150 | I | 9              | FRANCIS1 | 0.12204685D 01 | 0.79455716D-03 | 0.14701186D 02 |
| KE2150 |   | 0.12922126D 04 |          |                | 292 355        | 0.11D-03       |
| KE2155 | I | 4              | FRANCIS1 | 0.12095985D 01 | 0.79942029D-03 | 0.79448156D 01 |
| KE2155 |   | 0.24433069D 04 |          |                | 293 360        | 0.24D-03       |
| KE2170 | K | 2              | FRANCIS1 | 0.12807347D 01 | 0.86907800D-03 | 0.00000000D 00 |
| KE2170 |   | 0.00000000D 00 |          |                | 287 294        |                |
| KE2190 | K | 3              | FRANCIS1 | 0.16299756D 01 | 0.10330470D-02 | 0.00000000D 00 |
| KE2190 |   | 0.00000000D 00 |          |                | 362 407        |                |
| KE2225 | I | 6              | FRANCIS1 | 0.11714888D 01 | 0.66504418D-03 | 0.63866241D 02 |
| KE2225 |   | 0.22372144D 04 |          |                | 343 416        | 0.17D-03       |
| KE2235 | K | 3              | FRANCIS1 | 0.11643365D 01 | 0.87794400D-03 | 0.00000000D 00 |
| KE2235 |   | 0.00000000D 00 |          |                | 288 294        |                |
| KE2250 | I | 8              | FRANCIS1 | 0.11945877D 01 | 0.78531238D-03 | 0.15419426D 02 |
| KE2250 |   | 0.65498828D 04 |          |                | 299 354        | 0.13D-03       |
| KE2260 | I | 4              | FRANCIS1 | 0.13363056D 01 | 0.72387094D-03 | 0.21761551D 02 |
| KE2260 |   | 0.45346445D 04 |          |                | 293 359        | 0.26D-03       |
| KE2300 | I | 14             | FRANCIS1 | 0.10458326D 01 | 0.69680461D-03 | 0.47666807D 01 |
| KE2300 |   | 0.67093164D 03 |          |                | 303 434        | 0.28D-04       |
| KE2350 | I | 4              | FRANCIS1 | 0.11599350D 01 | 0.66308654D-03 | 0.26666517D 01 |
| KE2350 |   | 0.49937061D 03 |          |                | 294 354        | 0.12D-03       |
| KE2365 | H | 16             | FRANCIS1 | 0.13401823D 01 | 0.75588422D-03 | 0.45055351D 01 |
| KE2365 |   | 0.69762964D 03 |          |                | 328 524        | 0.21D-03       |
| KE2380 | I | 4              | FRANCIS1 | 0.13082275D 01 | 0.72633754D-03 | 0.51078349D-02 |
| KE2380 |   | 0.38099902D 03 |          |                | 293 359        | 0.23D-04       |
| KE2430 | I | 7              | FRANCIS1 | 0.14260750D 01 | 0.73180185D-03 | 0.32127676D 01 |
| KE2430 |   | 0.16007200D 04 |          |                | 403 461        | 0.72D-03       |
| KE2445 | I | 4              | FRANCIS1 | 0.12868528D 01 | 0.70454692D-03 | 0.12738742D 02 |
| KE2445 |   | 0.17073696D 04 |          |                | 293 359        | 0.38D-03       |
| KE2460 | K | 2              | FRANCIS1 | 0.15605904D 01 | 0.87257900D-03 | 0.00000000D 00 |
| KE2460 |   | 0.00000000D 00 |          |                | 565 576        |                |
| KE2506 | K | 3              | FRANCIS1 | 0.10552623D 01 | 0.76081000D-03 | 0.00000000D 00 |
| KE2506 |   | 0.00000000D 00 |          |                | 312 354        |                |
| KE2540 | I | 8              | FRANCIS1 | 0.11673403D 01 | 0.70211850D-03 | 0.19182373D 02 |
| KE2540 |   | 0.99052905D 03 |          |                | 293 354        | 0.10D-03       |
| KE2565 | I | 4              | FRANCIS1 | 0.12601871D 01 | 0.69377758D-03 | 0.52163324D 01 |
| KE2565 |   | 0.12629890D 04 |          |                | 293 359        | 0.11D-03       |
| KE2630 | I | 4              | FRANCIS1 | 0.13531923D 01 | 0.77704038D-03 | 0.37081345D 02 |
| KE2630 |   | 0.17556663D 04 |          |                | 348 407        | 0.29D-03       |
| KE2645 | I | 4              | FRANCIS1 | 0.12418633D 01 | 0.70035667D-03 | 0.49999952D-02 |
| KE2645 |   | 0.80786211D 04 |          |                | 293 359        | 0.23D-03       |
| KE2680 | J | 4              | FRANCIS1 | 0.15772915D 01 | 0.82694599D-03 | 0.15674782D 03 |
| KE2680 |   | 0.31303765D 04 |          |                | 367 427        | 0.41D-02       |
| KE2685 | I | 4              | FRANCIS1 | 0.17867718D 01 | 0.96267578D-03 | 0.19923569D 02 |
| KE2685 |   | 0.15690449D 04 |          |                | 346 409        | 0.82D-03       |
| KE2688 | I | 4              | FRANCIS1 | 0.15926456D 01 | 0.86395908D-03 | 0.50203278D 02 |
| KE2688 |   | 0.44107930D 04 |          |                | 367 423        | 0.84D-03       |
| KE2707 | K | 2              | FRANCIS1 | 0.10381524D 01 | 0.69986300D-03 | 0.00000000D 00 |
| KE2707 |   | 0.00000000D 00 |          |                | 333 354        |                |
| KE2745 | K | 3              | FRANCIS1 | 0.13130190D 01 | 0.71617300D-03 | 0.00000000D 00 |
| KE2745 |   | 0.00000000D 00 |          |                | 391 445        |                |

Table 14. Range 1 liquid density correlations--Continued

|        |   |                |          |                |                |                |
|--------|---|----------------|----------|----------------|----------------|----------------|
| KE2755 | I | 4              | FRANCIS1 | 0.12268534D 01 | 0.67655882D-03 | 0.18401814D 01 |
| KE2755 |   | 0.69340601D 03 |          |                | 293            | 359 0.49D-04   |
| KE2835 | I | 5              | FRANCIS1 | 0.11383848D 01 | 0.66913106D-03 | 0.49246109D 02 |
| KE2835 |   | 0.24330369D 04 |          |                | 319            | 357 0.15D-03   |
| KE2845 | I | 4              | FRANCIS1 | 0.12137480D 01 | 0.67674927D-03 | 0.45696878D 01 |
| KE2845 |   | 0.12091201D 04 |          |                | 293            | 359 0.89D-04   |
| KE3050 | I | 5              | FRANCIS1 | 0.11290541D 01 | 0.66905282D-03 | 0.51053818D 02 |
| KE3050 |   | 0.27560354D 04 |          |                | 328            | 355 0.14D-03   |
| KE3310 | K | 2              | FRANCIS1 | 0.10338106D 01 | 0.67308100D-03 | 0.00000000D 00 |
| KE3310 |   | 0.00000000D 00 |          |                | 343            | 365            |
| KE3350 | I | 5              | FRANCIS1 | 0.11021729D 01 | 0.68568555D-03 | 0.27912140D 00 |
| KE3350 |   | 0.60188306D 03 |          |                | 353            | 574 0.63D-03   |
| KE3712 | K | 2              | FRANCIS1 | 0.10227895D 01 | 0.63346800D-03 | 0.00000000D 00 |
| KE3712 |   | 0.00000000D 00 |          |                | 353            | 365            |
| KE4114 | J | 5              | FRANCIS1 | 0.10310059D 01 | 0.64559188D-03 | 0.19765949D 00 |
| KE4114 |   | 0.75869238D 03 |          |                | 363            | 574 0.13D-02   |
| KE4516 | K | 2              | FRANCIS1 | 0.10552416D 01 | 0.71184300D-03 | 0.00000000D 00 |
| KE4516 |   | 0.00000000D 00 |          |                | 361            | 369            |

Table 15. Range 2 liquid density correlations

|        |                |          |                |                |                  |
|--------|----------------|----------|----------------|----------------|------------------|
| KE0300 | A 34           | FRANCIS1 | 0.11081915D 01 | 0.10551438D-02 | 0.96902567D 00   |
| KE0300 | 0.40312988D 03 |          | 0.50809985D 03 |                | 178 330 0.20D-03 |
| KE0340 | K 3            | FRANCIS1 | 0.13919132D 01 | 0.10882850D-02 | 0.00000000D 00   |
| KE0340 | 0.00000000D 00 |          |                |                | 277 299          |
| KE0380 | H 12           | FRANCIS1 | 0.23480034D 01 | 0.25871226D-02 | 0.31269958D 02   |
| KE0380 | 0.42212915D 03 |          | 0.35713477D 03 |                | 210 295 0.14D-02 |
| KE0400 | G 47           | FRANCIS1 | 0.11104259D 01 | 0.81403158D-03 | 0.19753296D 02   |
| KE0400 | 0.58889380D 03 |          | 0.53677979D 03 |                | 195 324 0.17D-03 |
| KE0420 | I 13           | FRANCIS1 | 0.12236357D 01 | 0.87728817D-03 | 0.74975948D 01   |
| KE0420 | 0.52308423D 03 |          |                |                | 273 363 0.51D-03 |
| KE0430 | I 9            | FRANCIS1 | 0.14537134D 01 | 0.10908672D-02 | 0.14505398D 02   |
| KE0430 | 0.65764941D 03 |          |                |                | 282 303 0.14D-03 |
| KE0500 | H 9            | FRANCIS1 | 0.10936251D 01 | 0.96370699D-03 | 0.48774409D 00   |
| KE0500 | 0.42092505D 03 |          | 0.56107983D 03 |                | 233 354 0.11D-03 |
| KE0501 | H 19           | FRANCIS1 | 0.10943232D 01 | 0.86304802D-03 | 0.70360441D 01   |
| KE0501 | 0.55340259D 03 |          | 0.56145996D 03 |                | 273 348 0.66D-04 |
| KE0505 | K 3            | FRANCIS1 | 0.10588190D 01 | 0.84827400D-03 | 0.00000000D 00   |
| KE0505 | 0.00000000D 00 |          |                |                | 283 324          |
| KE0510 | H 27           | FRANCIS1 | 0.12644968D 01 | 0.89787156D-03 | 0.80934544D 01   |
| KE0510 | 0.61981030D 03 |          |                |                | 277 374 0.20D-03 |
| KE0520 | H 15           | FRANCIS1 | 0.12307463D 01 | 0.95416536D-03 | 0.36097822D 01   |
| KE0520 | 0.17891855D 04 |          |                |                | 273 364 0.12D-03 |
| KE0530 | I 4            | FRANCIS1 | 0.11695671D 01 | 0.90240128D-03 | 0.82282317D 00   |
| KE0530 | 0.43741748D 03 |          |                |                | 293 361 0.59D-04 |
| KE0540 | K 3            | FRANCIS1 | 0.11309113D 01 | 0.95017100D-03 | 0.00000000D 00   |
| KE0540 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0563 | K 2            | FRANCIS1 | 0.12291625D 01 | 0.82216200D-03 | 0.00000000D 00   |
| KE0563 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0568 | K 2            | FRANCIS1 | 0.14145337D 01 | 0.11002640D-02 | 0.00000000D 00   |
| KE0568 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0600 | H 7            | FRANCIS1 | 0.10629501D 01 | 0.76617324D-03 | 0.67085629D 01   |
| KE0600 | 0.54074902D 03 |          | 0.58700000D 03 |                | 283 334 0.18D-03 |
| KE0601 | I 4            | FRANCIS1 | 0.10622683D 01 | 0.75031724D-03 | 0.48805723D 01   |
| KE0601 | 0.47581445D 03 |          | 0.58281982D 03 |                | 297 324 0.14D-04 |
| KE0604 | H 18           | FRANCIS1 | 0.10666428D 01 | 0.82335575D-03 | 0.69826603D 01   |
| KE0604 | 0.57530029D 03 |          | 0.57100000D 03 |                | 273 374 0.11D-03 |
| KE0607 | I 13           | FRANCIS1 | 0.10912037D 01 | 0.94584492D-03 | 0.63908215D 01   |
| KE0607 | 0.12265347D 04 |          | 0.56700000D 03 |                | 293 354 0.29D-04 |
| KE0610 | K 2            | FRANCIS1 | 0.11699327D 01 | 0.67871500D-03 | 0.00000000D 00   |
| KE0610 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0615 | J 21           | FRANCIS1 | 0.12592354D 01 | 0.73114224D-03 | 0.24115524D 02   |
| KE0615 | 0.65499878D 03 |          |                |                | 277 374 0.51D-03 |
| KE0620 | H 15           | FRANCIS1 | 0.12110815D 01 | 0.84087066D-03 | 0.62623587D 01   |
| KE0620 | 0.64040259D 03 |          | 0.62900000D 03 |                | 273 354 0.49D-04 |
| KE0625 | K 3            | FRANCIS1 | 0.11754525D 01 | 0.89549800D-03 | 0.00000000D 00   |
| KE0625 | 0.00000000D 00 |          |                |                | 293 361          |
| KE0650 | I 6            | FRANCIS1 | 0.11541748D 01 | 0.92861406D-03 | 0.12769001D 02   |
| KE0650 | 0.83510986D 03 |          |                |                | 293 394 0.43D-04 |
| KE0660 | I 4            | FRANCIS1 | 0.15105515D 01 | 0.97980653D-03 | 0.19811020D 02   |
| KE0660 | 0.90835181D 03 |          |                |                | 395 434 0.17D-03 |
| KE0670 | I 6            | FRANCIS1 | 0.12066355D 01 | 0.88522420D-03 | 0.25476007D 01   |
| KE0670 | 0.59638232D 03 |          |                |                | 293 394 0.18D-03 |

Table 15. Range 2 liquid density correlations--Continued

|        |                |                |                |                  |
|--------|----------------|----------------|----------------|------------------|
| KE1040 | K 2 FRANCIS1   | 0.10481059D 01 | 0.76418900D-03 | 0.00000000D 00   |
| KE1040 | 0.00000000D 00 |                |                | 293 299          |
| KE1150 | I 4 FRANCIS1   | 0.11017246D 01 | 0.64413319D-03 | 0.50127020D 01   |
| KE1150 | 0.49241553D 03 |                |                | 303 363 0.56D-05 |
| KE1180 | I 4 FRANCIS1   | 0.12283163D 01 | 0.72272122D-03 | 0.87706625D 00   |
| KE1180 | 0.43193555D 03 |                |                | 293 359 0.10D-03 |
| KE1181 | I 7 FRANCIS1   | 0.12354736D 01 | 0.75112213D-03 | 0.29371872D 01   |
| KE1181 | 0.51115088D 03 |                |                | 293 359 0.28D-03 |
| KE1250 | I 9 FRANCIS1   | 0.13698235D 01 | 0.83868415D-03 | 0.96535120D 01   |
| KE1250 | 0.10811353D 04 |                |                | 313 354 0.22D-03 |
| KE1320 | K 2 FRANCIS1   | 0.11775263D 01 | 0.82878800D-03 | 0.00000000D 00   |
| KE1320 | 0.00000000D 00 |                |                | 289 294          |
| KE1350 | K 3 FRANCIS1   | 0.19414714D 01 | 0.12592340D-02 | 0.00000000D 00   |
| KE1350 | 0.00000000D 00 |                |                | 306 347          |
| KE1360 | K 3 FRANCIS1   | 0.14523771D 01 | 0.95708700D-03 | 0.00000000D 00   |
| KE1360 | 0.00000000D 00 |                |                | 292 362          |
| KE1400 | K 3 FRANCIS1   | 0.10606149D 01 | 0.80690800D-03 | 0.00000000D 00   |
| KE1400 | 0.00000000D 00 |                |                | 288 304          |
| KE1401 | I 4 FRANCIS1   | 0.10355082D 01 | 0.68153860D-03 | 0.24201708D 01   |
| KE1401 | 0.52146802D 03 |                |                | 293 359 0.71D-04 |
| KE1403 | K 3 FRANCIS1   | 0.10556330D 01 | 0.78969400D-03 | 0.00000000D 00   |
| KE1403 | 0.00000000D 00 |                |                | 297 324          |
| KE1530 | I 7 FRANCIS1   | 0.11216106D 01 | 0.75179804D-03 | 0.11565094D 01   |
| KE1530 | 0.58048584D 03 |                |                | 273 374 0.47D-04 |
| KE1550 | I 5 FRANCIS1   | 0.11585274D 01 | 0.88412291D-03 | 0.99014626D 01   |
| KE1550 | 0.11632017D 04 |                |                | 287 294 0.14D-04 |
| KE1580 | J 6 FRANCIS1   | 0.11929045D 01 | 0.71501243D-03 | 0.31916519D 02   |
| KE1580 | 0.73905195D 04 |                |                | 291 359 0.76D-03 |
| KE1620 | K 3 FRANCIS1   | 0.12227294D 01 | 0.85964500D-03 | 0.00000000D 00   |
| KE1620 | 0.00000000D 00 |                |                | 453 474          |
| KE1640 | K 3 FRANCIS1   | 0.11054682D 01 | 0.64550500D-03 | 0.00000000D 00   |
| KE1640 | 0.00000000D 00 |                |                | 286 294          |
| KE1660 | K 2 FRANCIS1   | 0.12286730D 01 | 0.10305550D-02 | 0.00000000D 00   |
| KE1660 | 0.00000000D 00 |                |                | 289 294          |
| KE1680 | K 2 FRANCIS1   | 0.12271983D 01 | 0.10002810D-02 | 0.00000000D 00   |
| KE1680 | 0.00000000D 00 |                |                | 288 294          |
| KE1750 | I 7 FRANCIS1   | 0.11910629D 01 | 0.65790350D-03 | 0.14866219D 01   |
| KE1750 | 0.44262402D 03 |                |                | 291 360 0.26D-03 |
| KE1760 | I 4 FRANCIS1   | 0.12143669D 01 | 0.77111414D-03 | 0.56137331D-01   |
| KE1760 | 0.37699731D 03 |                |                | 293 360 0.21D-04 |
| KE1762 | I 4 FRANCIS1   | 0.11962500D 01 | 0.70684613D-03 | 0.24943739D 00   |
| KE1762 | 0.39578760D 03 |                |                | 298 361 0.45D-06 |
| KE1860 | I 8 FRANCIS1   | 0.13859816D 01 | 0.94468961D-03 | 0.49999952D-02   |
| KE1860 | 0.49347217D 03 |                |                | 333 374 0.92D-03 |
| KE2000 | I 4 FRANCIS1   | 0.16353292D 01 | 0.10515784D-02 | 0.53056593D 01   |
| KE2000 | 0.85100244D 03 |                |                | 296 354 0.18D-03 |
| KE2100 | G 28 FRANCIS1  | 0.10617561D 01 | 0.66399807D-03 | 0.19551086D 02   |
| KE2100 | 0.76776074D 03 |                |                | 293 434 0.88D-04 |
| KE2104 | I 5 FRANCIS1   | 0.10162287D 01 | 0.57980116D-03 | 0.45092754D 01   |
| KE2104 | 0.50070825D 03 |                |                | 293 360 0.12D-03 |
| KE2120 | I 9 FRANCIS1   | 0.11690245D 01 | 0.72760601D-03 | 0.35297394D 01   |
| KE2120 | 0.16314060D 04 |                |                | 301 412 0.11D-03 |

Table 15. Range 2 liquid density correlations--Continued

|        |                |          |                |                |                  |
|--------|----------------|----------|----------------|----------------|------------------|
| KE0700 | G 16           | FRANCIS1 | 0.10823164D 01 | 0.68128319D-03 | 0.28077332D 02   |
| KE0700 | 0.71180640D 03 |          | 0.61150000D 03 |                | 288 429 0.10D-03 |
| KE0701 | I 7            | FRANCIS1 | 0.10566082D 01 | 0.76659396D-03 | 0.29826403D 01   |
| KE0701 | 0.51027295D 03 |          |                |                | 288 360 0.14D-03 |
| KE0702 | H 10           | FRANCIS1 | 0.10744505D 01 | 0.73973392D-03 | 0.12342205D 02   |
| KE0702 | 0.59130103D 03 |          |                |                | 253 394 0.41D-03 |
| KE0720 | G 24           | FRANCIS1 | 0.10650043D 01 | 0.79409732D-03 | 0.79816027D 01   |
| KE0720 | 0.59359106D 03 |          |                |                | 283 374 0.39D-03 |
| KE0725 | I 20           | FRANCIS1 | 0.12179537D 01 | 0.80069271D-03 | 0.10817964D 02   |
| KE0725 | 0.63199292D 03 |          |                |                | 288 374 0.18D-03 |
| KE0730 | I 18           | FRANCIS1 | 0.12222862D 01 | 0.81374589D-03 | 0.84028273D 01   |
| KE0730 | 0.60423389D 03 |          |                |                | 277 374 0.10D-03 |
| KE0735 | I 13           | FRANCIS1 | 0.13543797D 01 | 0.89812255D-03 | 0.94656706D 01   |
| KE0735 | 0.10463357D 04 |          |                |                | 313 374 0.31D-03 |
| KE0740 | I 7            | FRANCIS1 | 0.11986494D 01 | 0.81006484D-03 | 0.38449039D 01   |
| KE0740 | 0.65876953D 03 |          |                |                | 297 374 0.75D-04 |
| KE0745 | J 7            | FRANCIS1 | 0.11601934D 01 | 0.70832646D-03 | 0.10340004D 02   |
| KE0745 | 0.66066748D 03 |          |                |                | 292 357 0.14D-02 |
| KE0746 | J 6            | FRANCIS1 | 0.11473150D 01 | 0.77219424D-03 | 0.26848648D 02   |
| KE0746 | 0.44958086D 04 |          |                |                | 291 361 0.78D-03 |
| KE0747 | G 8            | FRANCIS1 | 0.11351528D 01 | 0.70543634D-03 | 0.90721703D 00   |
| KE0747 | 0.37699731D 03 |          |                |                | 291 360 0.37D-02 |
| KE0760 | I 5            | FRANCIS1 | 0.13968458D 01 | 0.88775204D-03 | 0.16219463D 01   |
| KE0760 | 0.61806470D 03 |          |                |                | 348 401 0.42D-03 |
| KE0800 | H 17           | FRANCIS1 | 0.10774565D 01 | 0.79408265D-03 | 0.89678802D 01   |
| KE0800 | 0.64906519D 03 |          |                |                | 253 434 0.26D-03 |
| KE0801 | I 6            | FRANCIS1 | 0.10447025D 01 | 0.75790938D-03 | 0.56298885D-01   |
| KE0801 | 0.37720679D 03 |          |                |                | 293 360 0.13D-03 |
| KE0802 | K 3            | FRANCIS1 | 0.10581158D 01 | 0.81718800D-03 | 0.00000000D 00   |
| KE0802 | 0.00000000D 00 |          |                |                | 297 324          |
| KE0850 | K 2            | FRANCIS1 | 0.10557714D 01 | 0.85020700D-03 | 0.00000000D 00   |
| KE0850 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0890 | I 8            | FRANCIS1 | 0.11752396D 01 | 0.74465154D-03 | 0.23469505D 01   |
| KE0890 | 0.55955298D 03 |          |                |                | 329 412 0.72D-04 |
| KE0910 | K 3            | FRANCIS1 | 0.11457132D 01 | 0.83233000D-03 | 0.00000000D 00   |
| KE0910 | 0.00000000D 00 |          |                |                | 273 294          |
| KE0930 | I 20           | FRANCIS1 | 0.12116728D 01 | 0.71956799D-03 | 0.64043417D 01   |
| KE0930 | 0.51158325D 03 |          |                |                | 277 374 0.13D-03 |
| KE0950 | H 17           | FRANCIS1 | 0.12849731D 01 | 0.82102115D-03 | 0.73394318D 01   |
| KE0950 | 0.74487476D 03 |          |                |                | 293 475 0.84D-04 |
| KE0980 | K 2            | FRANCIS1 | 0.14689927D 01 | 0.94420500D-03 | 0.00000000D 00   |
| KE0980 | 0.00000000D 00 |          |                |                | 293 299          |
| KE1000 | H 16           | FRANCIS1 | 0.10667076D 01 | 0.69098081D-03 | 0.18308731D 02   |
| KE1000 | 0.71997681D 03 |          |                |                | 298 439 0.74D-04 |
| KE1001 | J 4            | FRANCIS1 | 0.10525827D 01 | 0.76424866D-03 | 0.19214630D 02   |
| KE1001 | 0.30584688D 04 |          |                |                | 293 359 0.25D-02 |
| KE1002 | K 3            | FRANCIS1 | 0.10635706D 01 | 0.82080900D-03 | 0.00000000D 00   |
| KE1002 | 0.00000000D 00 |          |                |                | 297 324          |
| KE1003 | H 8            | FRANCIS1 | 0.10534096D 01 | 0.79098716D-03 | 0.49999952D-02   |
| KE1003 | 0.88935620D 03 |          | 0.64000000D 03 |                | 283 360 0.49D-03 |
| KE1020 | I 6            | FRANCIS1 | 0.10386066D 01 | 0.75689703D-03 | 0.34747953D 01   |
| KE1020 | 0.60697998D 03 |          |                |                | 293 359 0.22D-03 |

Table 15. Range 2 liquid density correlations--Continued

|        |                |    |          |                |                |                |
|--------|----------------|----|----------|----------------|----------------|----------------|
| KE2130 | I              | 4  | FRANCIS1 | 0.12822104D 01 | 0.88562258D-03 | 0.85805788D 01 |
| KE2130 | 0.38810552D 04 |    |          |                | 289 352        | 0.20D-03       |
| KE2150 | I              | 9  | FRANCIS1 | 0.12204685D 01 | 0.79455716D-03 | 0.14701186D 02 |
| KE2150 | 0.12922126D 04 |    |          |                | 292 355        | 0.11D-03       |
| KE2155 | I              | 4  | FRANCIS1 | 0.12095985D 01 | 0.79942029D-03 | 0.79448156D 01 |
| KE2155 | 0.24433069D 04 |    |          |                | 293 360        | 0.24D-03       |
| KE2170 | K              | 2  | FRANCIS1 | 0.12807347D 01 | 0.86907800D-03 | 0.00000000D 00 |
| KE2170 | 0.00000000D 00 |    |          |                | 287 294        |                |
| KE2190 | K              | 3  | FRANCIS1 | 0.16299756D 01 | 0.10330470D-02 | 0.00000000D 00 |
| KE2190 | 0.00000000D 00 |    |          |                | 362 407        |                |
| KE2225 | I              | 6  | FRANCIS1 | 0.11714888D 01 | 0.66504418D-03 | 0.63866241D 02 |
| KE2225 | 0.22372144D 04 |    |          |                | 343 416        | 0.17D-03       |
| KE2235 | K              | 3  | FRANCIS1 | 0.11643365D 01 | 0.87794400D-03 | 0.00000000D 00 |
| KE2235 | 0.00000000D 00 |    |          |                | 288 294        |                |
| KE2250 | I              | 8  | FRANCIS1 | 0.11945877D 01 | 0.78531238D-03 | 0.15419426D 02 |
| KE2250 | 0.65498828D 04 |    |          |                | 299 354        | 0.13D-03       |
| KE2260 | I              | 4  | FRANCIS1 | 0.13363056D 01 | 0.72387094D-03 | 0.21761551D 02 |
| KE2260 | 0.45346445D 04 |    |          |                | 293 359        | 0.26D-03       |
| KE2300 | I              | 14 | FRANCIS1 | 0.10458326D 01 | 0.69680461D-03 | 0.47666807D 01 |
| KE2300 | 0.67093164D 03 |    |          |                | 303 434        | 0.28D-04       |
| KE2350 | I              | 4  | FRANCIS1 | 0.11599350D 01 | 0.66308654D-03 | 0.26666517D 01 |
| KE2350 | 0.49937061D 03 |    |          |                | 294 354        | 0.12D-03       |
| KE2365 | H              | 16 | FRANCIS1 | 0.13401823D 01 | 0.75588422D-03 | 0.45055351D 01 |
| KE2365 | 0.69762964D 03 |    |          |                | 328 524        | 0.21D-03       |
| KE2380 | I              | 4  | FRANCIS1 | 0.13082275D 01 | 0.72633754D-03 | 0.51078349D-02 |
| KE2380 | 0.38099902D 03 |    |          |                | 293 359        | 0.23D-04       |
| KE2430 | I              | 7  | FRANCIS1 | 0.14260750D 01 | 0.73180185D-03 | 0.32127676D 01 |
| KE2430 | 0.16007200D 04 |    |          |                | 403 461        | 0.72D-03       |
| KE2445 | I              | 4  | FRANCIS1 | 0.12868528D 01 | 0.70454692D-03 | 0.12738742D 02 |
| KE2445 | 0.17073696D 04 |    |          |                | 293 359        | 0.38D-03       |
| KE2460 | K              | 2  | FRANCIS1 | 0.15605904D 01 | 0.87257900D-03 | 0.00000000D 00 |
| KE2460 | 0.00000000D 00 |    |          |                | 565 576        |                |
| KE2506 | K              | 3  | FRANCIS1 | 0.10552623D 01 | 0.76081000D-03 | 0.00000000D 00 |
| KE2506 | 0.00000000D 00 |    |          |                | 312 354        |                |
| KE2540 | I              | 8  | FRANCIS1 | 0.11673403D 01 | 0.70211850D-03 | 0.19182373D 02 |
| KE2540 | 0.99052905D 03 |    |          |                | 293 354        | 0.10D-03       |
| KE2565 | I              | 4  | FRANCIS1 | 0.12601871D 01 | 0.69377758D-03 | 0.52163324D 01 |
| KE2565 | 0.12629890D 04 |    |          |                | 293 359        | 0.11D-03       |
| KE2630 | I              | 4  | FRANCIS1 | 0.13531923D 01 | 0.77704038D-03 | 0.37081345D 02 |
| KE2630 | 0.17556663D 04 |    |          |                | 348 407        | 0.29D-03       |
| KE2645 | I              | 4  | FRANCIS1 | 0.12418633D 01 | 0.70035667D-03 | 0.49999952D-02 |
| KE2645 | 0.80786211D 04 |    |          |                | 293 359        | 0.23D-03       |
| KE2680 | J              | 4  | FRANCIS1 | 0.15772915D 01 | 0.82694599D-03 | 0.15674782D 03 |
| KE2680 | 0.31303765D 04 |    |          |                | 367 427        | 0.41D-02       |
| KE2685 | I              | 4  | FRANCIS1 | 0.17867718D 01 | 0.96267578D-03 | 0.19923569D 02 |
| KE2685 | 0.15690449D 04 |    |          |                | 346 409        | 0.82D-03       |
| KE2688 | I              | 4  | FRANCIS1 | 0.15926456D 01 | 0.86395908D-03 | 0.50203278D 02 |
| KE2688 | 0.44107930D 04 |    |          |                | 367 423        | 0.84D-03       |
| KE2707 | K              | 2  | FRANCIS1 | 0.10381524D 01 | 0.69986300D-03 | 0.00000000D 00 |
| KE2707 | 0.00000000D 00 |    |          |                | 333 354        |                |
| KE2745 | K              | 3  | FRANCIS1 | 0.13130190D 01 | 0.71617300D-03 | 0.00000000D 00 |
| KE2745 | 0.00000000D 00 |    |          |                | 391 445        |                |

Table 15. Range 2 liquid density correlations--Continued

|        |   |                |          |                |                |                  |
|--------|---|----------------|----------|----------------|----------------|------------------|
| KE2755 | I | 4              | FRANCIS1 | 0.12268534D 01 | 0.67655882D-03 | 0.18401814D 01   |
| KE2755 |   | 0.69340601D 03 |          |                |                | 293 359 0.49D-04 |
| KE2835 | I | 5              | FRANCIS1 | 0.11383848D 01 | 0.66913106D-03 | 0.49246109D 02   |
| KE2835 |   | 0.24330369D 04 |          |                |                | 319 357 0.15D-03 |
| KE2845 | I | 4              | FRANCIS1 | 0.12137480D 01 | 0.67674927D-03 | 0.45696878D 01   |
| KE2845 |   | 0.12091201D 04 |          |                |                | 293 359 0.89D-04 |
| KE3050 | I | 5              | FRANCIS1 | 0.11290541D 01 | 0.66905282D-03 | 0.51053818D 02   |
| KE3050 |   | 0.27560354D 04 |          |                |                | 328 355 0.14D-03 |
| KE3310 | K | 2              | FRANCIS1 | 0.10338106D 01 | 0.67308100D-03 | 0.00000000D 00   |
| KE3310 |   | 0.00000000D 00 |          |                |                | 343 365          |
| KE3350 | I | 5              | FRANCIS1 | 0.11021729D 01 | 0.68568555D-03 | 0.27912140D 00   |
| KE3350 |   | 0.60188306D 03 |          |                |                | 353 574 0.63D-03 |
| KE3712 | K | 2              | FRANCIS1 | 0.10227895D 01 | 0.63346800D-03 | 0.00000000D 00   |
| KE3712 |   | 0.00000000D 00 |          |                |                | 353 365          |
| KE4114 | J | 5              | FRANCIS1 | 0.10310059D 01 | 0.64559188D-03 | 0.19765949D 00   |
| KE4114 |   | 0.75869238D 03 |          |                |                | 363 574 0.13D-02 |
| KE4516 | K | 2              | FRANCIS1 | 0.10552416D 01 | 0.71184300D-03 | 0.00000000D 00   |
| KE4516 |   | 0.00000000D 00 |          |                |                | 361 369          |

Table 16. Range 3 liquid density correlations

|        |   |                |          |                |                |                  |
|--------|---|----------------|----------|----------------|----------------|------------------|
| KE0300 | D | 53             | FRANCIS1 | 0.11216850D 01 | 0.97801606D-03 | 0.12052504D 02   |
| KE0300 |   | 0.55959619D 03 |          | 0.50809985D 03 |                | 178 476 0.71D-03 |
| KE0340 | K | 3              | FRANCIS1 | 0.13919132D 01 | 0.10882850D-02 | 0.00000000D 00   |
| KE0340 |   | 0.00000000D 00 |          |                |                | 277 299          |
| KE0380 | H | 12             | FRANCIS1 | 0.23480034D 01 | 0.25871226D-02 | 0.31269958D 02   |
| KE0380 |   | 0.42212915D 03 |          | 0.35713477D 03 |                | 210 295 0.14D-02 |
| KE0400 | G | 47             | FRANCIS1 | 0.11104259D 01 | 0.81403158D-03 | 0.19753296D 02   |
| KE0400 |   | 0.58889380D 03 |          | 0.53677979D 03 |                | 195 324 0.17D-03 |
| KE0420 | I | 13             | FRANCIS1 | 0.12236357D 01 | 0.87728817D-03 | 0.74975948D 01   |
| KE0420 |   | 0.52308423D 03 |          |                |                | 273 363 0.51D-03 |
| KE0430 | I | 9              | FRANCIS1 | 0.14537134D 01 | 0.10908672D-02 | 0.14505398D 02   |
| KE0430 |   | 0.65764941D 03 |          |                |                | 282 303 0.14D-03 |
| KE0500 | H | 9              | FRANCIS1 | 0.10936251D 01 | 0.96370699D-03 | 0.48774409D 00   |
| KE0500 |   | 0.42092505D 03 |          | 0.56107983D 03 |                | 233 354 0.11D-03 |
| KE0501 | H | 19             | FRANCIS1 | 0.10943232D 01 | 0.86304802D-03 | 0.70360441D 01   |
| KE0501 |   | 0.55340259D 03 |          | 0.56145996D 03 |                | 273 348 0.66D-04 |
| KE0505 | K | 3              | FRANCIS1 | 0.10588190D 01 | 0.84827400D-03 | 0.00000000D 00   |
| KE0505 |   | 0.00000000D 00 |          |                |                | 283 324          |
| KE0510 | H | 27             | FRANCIS1 | 0.12644968D 01 | 0.89787156D-03 | 0.80934544D 01   |
| KE0510 |   | 0.61981030D 03 |          |                |                | 277 374 0.20D-03 |
| KE0520 | H | 15             | FRANCIS1 | 0.12307463D 01 | 0.95416536D-03 | 0.36097822D 01   |
| KE0520 |   | 0.17891855D 04 |          |                |                | 273 364 0.12D-03 |
| KE0530 | I | 4              | FRANCIS1 | 0.11695671D 01 | 0.90240128D-03 | 0.82282317D 00   |
| KE0530 |   | 0.43741748D 03 |          |                |                | 293 361 0.59D-04 |
| KE0540 | K | 3              | FRANCIS1 | 0.11309113D 01 | 0.95017100D-03 | 0.00000000D 00   |
| KE0540 |   | 0.00000000D 00 |          |                |                | 293 299          |
| KE0563 | K | 2              | FRANCIS1 | 0.12291625D 01 | 0.82216200D-03 | 0.00000000D 00   |
| KE0563 |   | 0.00000000D 00 |          |                |                | 293 299          |
| KE0568 | K | 2              | FRANCIS1 | 0.14145337D 01 | 0.11002640D-02 | 0.00000000D 00   |
| KE0568 |   | 0.00000000D 00 |          |                |                | 293 299          |
| KE0600 | H | 7              | FRANCIS1 | 0.10629501D 01 | 0.76617324D-03 | 0.67085629D 01   |
| KE0600 |   | 0.54074902D 03 |          | 0.58700000D 03 |                | 283 334 0.18D-03 |
| KE0601 | I | 4              | FRANCIS1 | 0.10622683D 01 | 0.75031724D-03 | 0.48805723D 01   |
| KE0601 |   | 0.47581445D 03 |          | 0.58281982D 03 |                | 297 324 0.14D-04 |
| KE0604 | H | 18             | FRANCIS1 | 0.10666428D 01 | 0.82335575D-03 | 0.69826603D 01   |
| KE0604 |   | 0.57530029D 03 |          | 0.57100000D 03 |                | 273 374 0.11D-03 |
| KE0607 | I | 13             | FRANCIS1 | 0.10912037D 01 | 0.94584492D-03 | 0.63908215D 01   |
| KE0607 |   | 0.12265347D 04 |          | 0.56700000D 03 |                | 293 354 0.29D-04 |
| KE0610 | K | 2              | FRANCIS1 | 0.11699327D 01 | 0.67871500D-03 | 0.00000000D 00   |
| KE0610 |   | 0.00000000D 00 |          |                |                | 293 299          |
| KE0615 | J | 21             | FRANCIS1 | 0.12592354D 01 | 0.73114224D-03 | 0.24115524D 02   |
| KE0615 |   | 0.65499878D 03 |          |                |                | 277 374 0.51D-03 |
| KE0620 | H | 15             | FRANCIS1 | 0.12110815D 01 | 0.84087066D-03 | 0.62623587D 01   |
| KE0620 |   | 0.64040259D 03 |          | 0.62900000D 03 |                | 273 354 0.49D-04 |
| KE0625 | K | 3              | FRANCIS1 | 0.11754525D 01 | 0.89549800D-03 | 0.00000000D 00   |
| KE0625 |   | 0.00000000D 00 |          |                |                | 293 361          |
| KE0650 | I | 6              | FRANCIS1 | 0.11541748D 01 | 0.92861406D-03 | 0.12769001D 02   |
| KE0650 |   | 0.83510986D 03 |          |                |                | 293 394 0.43D-04 |
| KE0660 | I | 4              | FRANCIS1 | 0.15105515D 01 | 0.97980653D-03 | 0.19811020D 02   |
| KE0660 |   | 0.90835181D 03 |          |                |                | 395 434 0.17D-03 |
| KE0670 | I | 6              | FRANCIS1 | 0.12066355D 01 | 0.88522420D-03 | 0.25476007D 01   |
| KE0670 |   | 0.59638232D 03 |          |                |                | 293 394 0.18D-03 |

Table 16. Range 3 liquid density correlations--Continued

|        |                |          |                |                |                  |
|--------|----------------|----------|----------------|----------------|------------------|
| KE0700 | G 16           | FRANCIS1 | 0.10823164D 01 | 0.68128319D-03 | 0.28077332D 02   |
| KE0700 | 0.71180640D 03 |          | 0.61150000D 03 |                | 288 429 0.10D-03 |
| KE0701 | I 7            | FRANCIS1 | 0.10566082D 01 | 0.76659396D-03 | 0.29826403D 01   |
| KE0701 | 0.51027295D 03 |          |                |                | 288 360 0.14D-03 |
| KE0702 | H 10           | FRANCIS1 | 0.10744505D 01 | 0.73973392D-03 | 0.12342205D 02   |
| KE0702 | 0.59130103D 03 |          |                |                | 253 394 0.41D-03 |
| KE0720 | G 24           | FRANCIS1 | 0.10650043D 01 | 0.79409732D-03 | 0.79816027D 01   |
| KE0720 | 0.59359106D 03 |          |                |                | 283 374 0.39D-03 |
| KE0725 | I 20           | FRANCIS1 | 0.12179537D 01 | 0.80069271D-03 | 0.10817964D 02   |
| KE0725 | 0.63199292D 03 |          |                |                | 288 374 0.18D-03 |
| KE0730 | I 18           | FRANCIS1 | 0.12222862D 01 | 0.81374589D-03 | 0.84028273D 01   |
| KE0730 | 0.60423389D 03 |          |                |                | 277 374 0.10D-03 |
| KE0735 | I 13           | FRANCIS1 | 0.13543797D 01 | 0.89812255D-03 | 0.94656706D 01   |
| KE0735 | 0.10463357D 04 |          |                |                | 313 374 0.31D-03 |
| KE0740 | I 7            | FRANCIS1 | 0.11986494D 01 | 0.81006484D-03 | 0.38449039D 01   |
| KE0740 | 0.65876953D 03 |          |                |                | 297 374 0.75D-04 |
| KE0745 | J 7            | FRANCIS1 | 0.11601934D 01 | 0.70832646D-03 | 0.10340004D 02   |
| KE0745 | 0.66066748D 03 |          |                |                | 292 357 0.14D-02 |
| KE0746 | J 6            | FRANCIS1 | 0.11473150D 01 | 0.77219424D-03 | 0.26848648D 02   |
| KE0746 | 0.44958086D 04 |          |                |                | 291 361 0.78D-03 |
| KE0747 | G 8            | FRANCIS1 | 0.11351528D 01 | 0.70543634D-03 | 0.90721703D 00   |
| KE0747 | 0.37699731D 03 |          |                |                | 291 360 0.37D-02 |
| KE0760 | I 5            | FRANCIS1 | 0.13968458D 01 | 0.88775204D-03 | 0.16219463D 01   |
| KE0760 | 0.61806470D 03 |          |                |                | 348 401 0.42D-03 |
| KE0800 | H 17           | FRANCIS1 | 0.10774565D 01 | 0.79408265D-03 | 0.89678802D 01   |
| KE0800 | 0.64906519D 03 |          |                |                | 253 434 0.26D-03 |
| KE0801 | I 6            | FRANCIS1 | 0.10447025D 01 | 0.75790938D-03 | 0.56298885D-01   |
| KE0801 | 0.37720679D 03 |          |                |                | 293 360 0.13D-03 |
| KE0802 | K 3            | FRANCIS1 | 0.10581158D 01 | 0.81718800D-03 | 0.00000000D 00   |
| KE0802 | 0.00000000D 00 |          |                |                | 297 324          |
| KE0850 | K 2            | FRANCIS1 | 0.10557714D 01 | 0.85020700D-03 | 0.00000000D 00   |
| KE0850 | 0.00000000D 00 |          |                |                | 293 299          |
| KE0890 | I 8            | FRANCIS1 | 0.11752396D 01 | 0.74465154D-03 | 0.23469505D 01   |
| KE0890 | 0.55955298D 03 |          |                |                | 329 412 0.72D-04 |
| KE0910 | K 3            | FRANCIS1 | 0.11457132D 01 | 0.83233000D-03 | 0.00000000D 00   |
| KE0910 | 0.00000000D 00 |          |                |                | 273 294          |
| KE0930 | I 20           | FRANCIS1 | 0.12116728D 01 | 0.71956799D-03 | 0.64043417D 01   |
| KE0930 | 0.51158325D 03 |          |                |                | 277 374 0.13D-03 |
| KE0950 | H 17           | FRANCIS1 | 0.12849731D 01 | 0.82102115D-03 | 0.73394318D 01   |
| KE0950 | 0.74487476D 03 |          |                |                | 293 475 0.84D-04 |
| KE0980 | K 2            | FRANCIS1 | 0.14689927D 01 | 0.94420500D-03 | 0.00000000D 00   |
| KE0980 | 0.00000000D 00 |          |                |                | 293 299          |
| KE1000 | H 16           | FRANCIS1 | 0.10667076D 01 | 0.69098081D-03 | 0.18308731D 02   |
| KE1000 | 0.71997681D 03 |          |                |                | 298 439 0.74D-04 |
| KE1001 | J 4            | FRANCIS1 | 0.10525827D 01 | 0.76424866D-03 | 0.19214630D 02   |
| KE1001 | 0.30584688D 04 |          |                |                | 293 359 0.25D-02 |
| KE1002 | K 3            | FRANCIS1 | 0.10635706D 01 | 0.82080900D-03 | 0.00000000D 00   |
| KE1002 | 0.00000000D 00 |          |                |                | 297 324          |
| KE1003 | H 8            | FRANCIS1 | 0.10534096D 01 | 0.79098716D-03 | 0.49999952D-02   |
| KE1003 | 0.88935620D 03 |          | 0.64000000D 03 |                | 283 360 0.49D-03 |
| KE1020 | I 6            | FRANCIS1 | 0.10386066D 01 | 0.75689703D-03 | 0.34747953D 01   |
| KE1020 | 0.60697998D 03 |          |                |                | 293 359 0.22D-03 |

Table 16. Range 3 liquid density correlations--Continued

|        |                |                |                |                  |
|--------|----------------|----------------|----------------|------------------|
| KE1040 | K 2 FRANCIS1   | 0.10481059D 01 | 0.76418900D-03 | 0.00000000D 00   |
| KE1040 | 0.00000000D 00 |                |                | 293 299          |
| KE1150 | I 4 FRANCIS1   | 0.11017246D 01 | 0.64413319D-03 | 0.50127020D 01   |
| KE1150 | 0.49241553D 03 |                |                | 303 363 0.56D-05 |
| KE1180 | I 4 FRANCIS1   | 0.12283163D 01 | 0.72272122D-03 | 0.87706625D 00   |
| KE1180 | 0.43193555D 03 |                |                | 293 359 0.10D-03 |
| KE1181 | I 7 FRANCIS1   | 0.12354736D 01 | 0.75112213D-03 | 0.29371872D 01   |
| KE1181 | 0.51115088D 03 |                |                | 293 359 0.28D-03 |
| KE1250 | I 9 FRANCIS1   | 0.13698235D 01 | 0.83868415D-03 | 0.96535120D 01   |
| KE1250 | 0.10811353D 04 |                |                | 313 354 0.22D-03 |
| KE1320 | K 2 FRANCIS1   | 0.11775263D 01 | 0.82878800D-03 | 0.00000000D 00   |
| KE1320 | 0.00000000D 00 |                |                | 289 294          |
| KE1350 | K 3 FRANCIS1   | 0.19414714D 01 | 0.12592340D-02 | 0.00000000D 00   |
| KE1350 | 0.00000000D 00 |                |                | 306 347          |
| KE1360 | K 3 FRANCIS1   | 0.14523771D 01 | 0.95708700D-03 | 0.00000000D 00   |
| KE1360 | 0.00000000D 00 |                |                | 292 362          |
| KE1400 | K 3 FRANCIS1   | 0.10606149D 01 | 0.80690800D-03 | 0.00000000D 00   |
| KE1400 | 0.00000000D 00 |                |                | 288 304          |
| KE1401 | I 4 FRANCIS1   | 0.10355082D 01 | 0.68153860D-03 | 0.24201708D 01   |
| KE1401 | 0.52146802D 03 |                |                | 293 359 0.71D-04 |
| KE1403 | K 3 FRANCIS1   | 0.10556330D 01 | 0.78969400D-03 | 0.00000000D 00   |
| KE1403 | 0.00000000D 00 |                |                | 297 324          |
| KE1530 | I 7 FRANCIS1   | 0.11216106D 01 | 0.75179804D-03 | 0.11565094D 01   |
| KE1530 | 0.58048584D 03 |                |                | 273 374 0.47D-04 |
| KE1550 | I 5 FRANCIS1   | 0.11585274D 01 | 0.88412291D-03 | 0.99014626D 01   |
| KE1550 | 0.11632017D 04 |                |                | 287 294 0.14D-04 |
| KE1580 | J 6 FRANCIS1   | 0.11929045D 01 | 0.71501243D-03 | 0.31916519D 02   |
| KE1580 | 0.73905195D 04 |                |                | 291 359 0.76D-03 |
| KE1620 | K 3 FRANCIS1   | 0.12227294D 01 | 0.85964500D-03 | 0.00000000D 00   |
| KE1620 | 0.00000000D 00 |                |                | 453 474          |
| KE1640 | K 3 FRANCIS1   | 0.11054682D 01 | 0.64550500D-03 | 0.00000000D 00   |
| KE1640 | 0.00000000D 00 |                |                | 286 294          |
| KE1660 | K 2 FRANCIS1   | 0.12286730D 01 | 0.10305550D-02 | 0.00000000D 00   |
| KE1660 | 0.00000000D 00 |                |                | 289 294          |
| KE1680 | K 2 FRANCIS1   | 0.12271983D 01 | 0.10002810D-02 | 0.00000000D 00   |
| KE1680 | 0.00000000D 00 |                |                | 288 294          |
| KE1750 | I 7 FRANCIS1   | 0.11910629D 01 | 0.65790350D-03 | 0.14866219D 01   |
| KE1750 | 0.44262402D 03 |                |                | 291 360 0.26D-03 |
| KE1760 | I 4 FRANCIS1   | 0.12143669D 01 | 0.77111414D-03 | 0.56137331D-01   |
| KE1760 | 0.37699731D 03 |                |                | 293 360 0.21D-04 |
| KE1762 | I 4 FRANCIS1   | 0.11962500D 01 | 0.70684613D-03 | 0.24943739D 00   |
| KE1762 | 0.39578760D 03 |                |                | 298 361 0.45D-06 |
| KE1860 | I 8 FRANCIS1   | 0.13859816D 01 | 0.94468961D-03 | 0.49999952D-02   |
| KE1860 | 0.49347217D 03 |                |                | 333 374 0.92D-03 |
| KE2000 | I 4 FRANCIS1   | 0.16353292D 01 | 0.10515784D-02 | 0.53056593D 01   |
| KE2000 | 0.85100244D 03 |                |                | 296 354 0.18D-03 |
| KE2100 | G 28 FRANCIS1  | 0.10617561D 01 | 0.66399807D-03 | 0.19551086D 02   |
| KE2100 | 0.76776074D 03 |                |                | 293 434 0.88D-04 |
| KE2104 | I 5 FRANCIS1   | 0.10162287D 01 | 0.57980116D-03 | 0.45092754D 01   |
| KE2104 | 0.50070825D 03 |                |                | 293 360 0.12D-03 |
| KE2120 | I 9 FRANCIS1   | 0.11690245D 01 | 0.72760601D-03 | 0.35297394D 01   |
| KE2120 | 0.16314060D 04 |                |                | 301 412 0.11D-03 |

Table 16. Range 3 liquid density correlations--Continued

|        |                |                |                |                  |
|--------|----------------|----------------|----------------|------------------|
| KE2130 | I 4 FRANCIS1   | 0.12822104D 01 | 0.88562258D-03 | 0.85805788D 01   |
| KE2130 | 0.38810552D 04 |                |                | 289 352 0.20D-03 |
| KE2150 | I 9 FRANCIS1   | 0.12204685D 01 | 0.79455716D-03 | 0.14701186D 02   |
| KE2150 | 0.12922126D 04 |                |                | 292 355 0.11D-03 |
| KE2155 | I 4 FRANCIS1   | 0.12095985D 01 | 0.79942029D-03 | 0.79448156D 01   |
| KE2155 | 0.24433069D 04 |                |                | 293 360 0.24D-03 |
| KE2170 | K 2 FRANCIS1   | 0.12807347D 01 | 0.86907800D-03 | 0.00000000D 00   |
| KE2170 | 0.00000000D 00 |                |                | 287 294          |
| KE2190 | K 3 FRANCIS1   | 0.16299756D 01 | 0.10330470D-02 | 0.00000000D 00   |
| KE2190 | 0.00000000D 00 |                |                | 362 407          |
| KE2225 | I 6 FRANCIS1   | 0.11714888D 01 | 0.66504418D-03 | 0.63866241D 02   |
| KE2225 | 0.22372144D 04 |                |                | 343 416 0.17D-03 |
| KE2235 | K 3 FRANCIS1   | 0.11643365D 01 | 0.87794400D-03 | 0.00000000D 00   |
| KE2235 | 0.00000000D 00 |                |                | 288 294          |
| KE2250 | I 8 FRANCIS1   | 0.11945877D 01 | 0.78531238D-03 | 0.15419426D 02   |
| KE2250 | 0.65498828D 04 |                |                | 299 354 0.13D-03 |
| KE2260 | I 4 FRANCIS1   | 0.13363056D 01 | 0.72387094D-03 | 0.21761551D 02   |
| KE2260 | 0.45346445D 04 |                |                | 293 359 0.26D-03 |
| KE2300 | I 14 FRANCIS1  | 0.10458326D 01 | 0.69680461D-03 | 0.47666807D 01   |
| KE2300 | 0.67093164D 03 |                |                | 303 434 0.28D-04 |
| KE2350 | I 4 FRANCIS1   | 0.11599350D 01 | 0.66308654D-03 | 0.26666517D 01   |
| KE2350 | 0.49937061D 03 |                |                | 294 354 0.12D-03 |
| KE2365 | H 16 FRANCIS1  | 0.13401823D 01 | 0.75588422D-03 | 0.45055351D 01   |
| KE2365 | 0.69762964D 03 |                |                | 328 524 0.21D-03 |
| KE2380 | I 4 FRANCIS1   | 0.13082275D 01 | 0.72633754D-03 | 0.51078349D-02   |
| KE2380 | 0.38099902D 03 |                |                | 293 359 0.23D-04 |
| KE2430 | I 7 FRANCIS1   | 0.14260750D 01 | 0.73180185D-03 | 0.32127676D 01   |
| KE2430 | 0.16007200D 04 |                |                | 403 461 0.72D-03 |
| KE2445 | I 4 FRANCIS1   | 0.12868528D 01 | 0.70454692D-03 | 0.12738742D 02   |
| KE2445 | 0.17073696D 04 |                |                | 293 359 0.38D-03 |
| KE2460 | K 2 FRANCIS1   | 0.15605904D 01 | 0.87257900D-03 | 0.00000000D 00   |
| KE2460 | 0.00000000D 00 |                |                | 565 576          |
| KE2506 | K 3 FRANCIS1   | 0.10552623D 01 | 0.76081000D-03 | 0.00000000D 00   |
| KE2506 | 0.00000000D 00 |                |                | 312 354          |
| KE2540 | I 8 FRANCIS1   | 0.11673403D 01 | 0.70211850D-03 | 0.19182373D 02   |
| KE2540 | 0.99052905D 03 |                |                | 293 354 0.10D-03 |
| KE2565 | I 4 FRANCIS1   | 0.12601871D 01 | 0.69377758D-03 | 0.52163324D 01   |
| KE2565 | 0.12629890D 04 |                |                | 293 359 0.11D-03 |
| KE2630 | I 4 FRANCIS1   | 0.13531923D 01 | 0.77704038D-03 | 0.37081345D 02   |
| KE2630 | 0.17556663D 04 |                |                | 348 407 0.29D-03 |
| KE2645 | I 4 FRANCIS1   | 0.12418633D 01 | 0.70035667D-03 | 0.49999952D-02   |
| KE2645 | 0.80786211D 04 |                |                | 293 359 0.23D-03 |
| KE2680 | J 4 FRANCIS1   | 0.15772915D 01 | 0.82694599D-03 | 0.15674782D 03   |
| KE2680 | 0.31303765D 04 |                |                | 367 427 0.41D-02 |
| KE2685 | I 4 FRANCIS1   | 0.17867718D 01 | 0.96267578D-03 | 0.19923569D 02   |
| KE2685 | 0.15690449D 04 |                |                | 346 409 0.82D-03 |
| KE2688 | I 4 FRANCIS1   | 0.15926456D 01 | 0.86395908D-03 | 0.50203278D 02   |
| KE2688 | 0.44107930D 04 |                |                | 367 423 0.84D-03 |
| KE2707 | K 2 FRANCIS1   | 0.10381524D 01 | 0.69986300D-03 | 0.00000000D 00   |
| KE2707 | 0.00000000D 00 |                |                | 333 354          |
| KE2745 | K 3 FRANCIS1   | 0.13130190D 01 | 0.71617300D-03 | 0.00000000D 00   |
| KE2745 | 0.00000000D 00 |                |                | 391 445          |

Table 16. Range 3 liquid density correlations--Continued

|        |   |                |          |                |                |                |
|--------|---|----------------|----------|----------------|----------------|----------------|
| KE2755 | I | 4              | FRANCIS1 | 0.12268534D 01 | 0.67655882D-03 | 0.18401814D 01 |
| KE2755 |   | 0.69340601D 03 |          |                | 293 359        | 0.49D-04       |
| KE2835 | I | 5              | FRANCIS1 | 0.11383848D 01 | 0.66913106D-03 | 0.49246109D 02 |
| KE2835 |   | 0.24330369D 04 |          |                | 319 357        | 0.15D-03       |
| KE2845 | I | 4              | FRANCIS1 | 0.12137480D 01 | 0.67674927D-03 | 0.45696878D 01 |
| KE2845 |   | 0.12091201D 04 |          |                | 293 359        | 0.89D-04       |
| KE3050 | I | 5              | FRANCIS1 | 0.11290541D 01 | 0.66905282D-03 | 0.51053818D 02 |
| KE3050 |   | 0.27560354D 04 |          |                | 328 355        | 0.14D-03       |
| KE3310 | K | 2              | FRANCIS1 | 0.10338106D 01 | 0.67308100D-03 | 0.00000000D 00 |
| KE3310 |   | 0.00000000D 00 |          |                | 343 365        |                |
| KE3350 | I | 5              | FRANCIS1 | 0.11021729D 01 | 0.68568555D-03 | 0.27912140D 00 |
| KE3350 |   | 0.60188306D 03 |          |                | 353 574        | 0.63D-03       |
| KE3712 | K | 2              | FRANCIS1 | 0.10227895D 01 | 0.63346800D-03 | 0.00000000D 00 |
| KE3712 |   | 0.00000000D 00 |          |                | 353 365        |                |
| KE4114 | J | 5              | FRANCIS1 | 0.10310059D 01 | 0.64559188D-03 | 0.19765949D 00 |
| KE4114 |   | 0.75869238D 03 |          |                | 363 574        | 0.13D-02       |
| KE4516 | K | 2              | FRANCIS1 | 0.10552416D 01 | 0.71184300D-03 | 0.00000000D 00 |
| KE4516 |   | 0.00000000D 00 |          |                | 361 369        |                |

Table 17. Range 4 liquid density correlations

|        |   |    |          |                |                |                |          |
|--------|---|----|----------|----------------|----------------|----------------|----------|
| KE0300 | H | 13 | FRANCIS2 | 0.11984767D-02 | 0.22339842D 01 | 0.27800000D 00 |          |
| KE0300 |   |    |          | 0.50809985D 03 | 460            | 508            | 0.26D-02 |

The last three items are the same as in the vapor pressure tables. The lower and upper temperature limits define the range of the experimental data points actually fitted by the correlation. The rmsd values are much better behaved than for vapor pressure due to the small numerical range covered by the liquid density, and are therefore easier to use in judging the scatter of the data points fitted in a given correlation.

As in the case of vapor pressure, a superficial judging of the quality of a correlation should be based on the quality rating primarily, with the number of points fitted and the rmsd value considered next in that order.

#### 5.4. Second Virial Coefficient

The quality ratings defined in Table 13 are not as useful for the second virial coefficient correlations as for the vapor pressure and liquid density. As explained in section 4.4, the literature data are not screened and no final selected set of data points is fitted to a selected correlation equation. Instead, a curve predicted by each of six predictive equations is "drawn" through all the available literature data sets for each compound. Table 4 shows how well each predictive equation agreed with each literature data set for the various ketones for which second virial coefficient data have been measured. The Tsonopoulos correlation [11414] was chosen for all those compounds except 2-butanone (KE0400) for which the Hayden-O'Connell [8531] correlation appeared to be slightly better.

The parameters for the Tsonopoulos equation for all those ketones with  $T_c$ ,  $P_c$ , acentric factor and dipole moment values are listed in Table 18. The first tier of compounds are those for which experimental B values were available for checking the accuracy level of the Tsonopoulos equation. (See table 4.) The second tier lists compounds for which no experimental B data are available but for which the availability of  $T_c$ ,  $P_c$ ,  $\omega$  and  $\mu$  values makes possible predictions with the Tsonopoulos equation. Based on the performance of that equation for the compounds in the first tier, there is a good probability that the B values predicted for the second tier of compounds will be close enough to be useful.

The Hayden-O'Connell parameters used for 2-butanone were as follows:

$T_c = 533.0 \text{ K}$ ,  $P_c = 39.50 \text{ atm}$ ,  $\mu = 2.70 \text{ Debye}$ ,  $\eta = 0.9$ ,  $R_D = 3.139 \text{ }^{\circ}\text{A}$ . These parameters were taken from the Hayden-O-Connell article [8531] and therefore differ in some instances from the values listed for 2-butanone in table 7.

#### 6.0 Equations of State

The uses which can be made of the vapor pressure and liquid density data are severely limited if a reliable equation of state is not available for the compound. Unfortunately, all the equations of state require the availability of  $T_c$  and  $P_c$  which limits their use to only a few compounds.

Table 18. Parameters used in the Tsonopoulos equation

| ID                  | T <sub>c</sub> , K | P <sub>c</sub> , atm | $\omega$ | a        | b   |
|---------------------|--------------------|----------------------|----------|----------|-----|
| KE0300              | 508.100            | 46.390               | 0.3073   | -0.0301  | 0.0 |
| KE0400              | 536.780            | 41.520               | 0.3220   | -0.0228  | 0.0 |
| KE0500              | 561.080            | 36.460               | 0.3470   | -0.0176  | 0.0 |
| KE0501              | 561.460            | 36.800               | 0.3410   | -0.0177  | 0.0 |
| KE0505              | 553.400            | 38.000               | 0.3301   | -0.0195  | 0.0 |
| KE0601 <sup>a</sup> | 582.820            | 32.770               | 0.3794   | -0.0142  | 0.0 |
| KE0600              | 587.000            | 32.795               | 0.3942   | -0.0140  | 0.0 |
| KE0604 <sup>a</sup> | 571.000            | 32.272               | 0.3663   | -0.0150  | 0.0 |
| KE0607              | 567.000            | 34.246               | 0.3229   | -0.0172  | 0.0 |
| KE0620              | 629.000            | 37.997               | 0.4524   | -0.0187  | 0.0 |
| KE0700              | 611.500            | 33.911               | 0.4857   | -0.0127  | 0.0 |
| KE1003              | 640.000            | 22.897               | 0.5138   | -0.00829 | 0.0 |

<sup>a</sup>Assumed values of 2.68 for KE0601 and 2.72 for KE0604 were used for the dipole moments.

An attempt is made to store in the pure compound data bank constants for three types of equations of state:

1. Benedict-Webb-Rubin. The original BWR equation [1339], the Sood and Haselden modification [9203], and the Starling modification [1794] can all be used.
2. Redlich-Kwong. The original Redlich-Kwong equation [1454], the Chueh-Prausnitz modification [7541], and the Lu modification [40370] are all supported. The Peng-Robinson equation [40275] is also used and is listed here because of its similarity to the Redlich-Kwong equation.
3. Virial. Space is assigned in the data bank for correlations for both the second and third virial coefficients. Those equations used for B are discussed in section 4.4. Up to the present time, the space for the C correlation has not been used because of the lack of C data and the lack of a reliable correlation equation.

No BWR constants are available for the ketones. Constants are not available for the Chueh-Prausnitz and the Lu modifications of the Redlich-Kwong. Rather than use the unmodified Redlich-Kwong equation for those compounds with  $T_c$  and  $P_c$  values, the Peng-Robinson equation could be used instead because the acentric factor was also available for all those compounds: KE0300, KE0370, KE0380, KE0400, KE0500, KE0501, KE0505, KE0600, KE0604, KE0607, KE0620, KE0700, KE1003. The  $T_c$ ,  $P_c$  and  $\omega$  values appear in table 7.

## 7. Data Tabulations

As a final check on the selected data before it is loaded into the pure compound data bank, program RECAL is used to produce data tabulations for proofing purposes. When satisfactory tables have been produced for all the compounds, the selected data are loaded into the pure compound data bank where it can be accessed via either interactive or batch programs.

Copies of the RECAL data tabulations for the 157 ketones for which some storable data were found can be purchased for \$200 by sending a check or a purchase order number along with a request for one set of the ketone tables to the Director, Thermodynamics Research Laboratory, Box 1144, Washington University, St. Louis, Missouri 63130. The entire set of ketone tables must be ordered; requests for individual tables will not be processed. A description of a compound table follows.

The first page lists the compound constants available for the compound. Below that tabulation, the values of the conversion constants used to convert the literature data values to the units used in the tables are given. The units used for the tables are kelvin, kilopascals, cubic centimeter/mole and joule/mole.

The tabulations of the temperature-dependent properties are split into the following three temperature intervals,

Interval 1       $T_m$  to  $(T_b + 10)$

Interval 2       $(T_b + 5)$  to  $(T_c - 40)$

Interval 3       $(T_c - 45)$  to  $T_c$

in order to best utilize the most accurate of the various temperature range fits defined in sections 4.2.3 and 4.3.3. The range fits used for each interval are as follows.

| <u>Interval</u> | <u>Property</u> | <u>Range fit</u> |
|-----------------|-----------------|------------------|
| 1               | vapor pressure  | range 2          |
|                 | liquid density  | range 2          |
| 2               | vapor pressure  | range 4          |
|                 | liquid density  | range 3          |
| 3               | vapor pressure  | range 4          |
|                 | liquid density  | range 4          |

For each interval, the following properties are tabulated at 1.0 K intervals when the necessary information is available: vapor pressure, saturated liquid volume, second virial coefficient, heat of vaporization and saturated vapor volume. Each of the first three requires that a correlation be available and that the specific temperature being listed falls within the range of the correlation being used. If a second virial coefficient correlation is stored

for the compound, a B value will be printed for all temperatures listed because no temperature limits are stored with the correlation equation constants. The heat of vaporization listed is calculated from the Clapeyron equation and listed when vapor pressure and saturated liquid density values are available, and an equation of state is available to provide the saturated vapor molar volume. If an equation of state and the vapor pressure are available, the saturated vapor molar volume will be calculated and listed.

Following the data tabulation for each of the three intervals, the equations used for that interval are printed along with their constants. The temperature limits, the number of data points fitted and the root-mean-squared deviation are given for each vapor pressure and liquid density equation. The second virial coefficient correlation is printed (if one is available) but no temperature limits, number of points, or root-mean-squared-deviation are given. The name of the equation of state used for the interval calculations is given but the equation itself is not printed. The best equation of state for an interval is chosen by program RECVAL by matching a hierarchy of choices against what is available in the compound data files. For the ketones, the virial and/or the Peng-Robinson equations of state were available for those compounds listed in sections 5.4 and 6.0. Equation of state calculations were made only if one or the other of those equations were available; i.e., the ideal gas equation of state was not used as a default.

The last pages of each compound table list the literature reference numbers associated with each property correlation. For the vapor pressure and liquid density correlations, the lists are split into two parts--the documents used and the documents not used for the correlation. A literature document is listed as a "used" document if it contributed at least one data point to the experimental data base upon which the correlation is based. The breakdown between used and not used documents is not necessary for the second virial coefficient correlation.

The used and not used reference numbers appearing at the end of a compound table are those which appear in Table 19 for that compound.

## 8. References

Table 19 identifies the literature documents which contain data for the various compound-property combinations. The compound is identified in the first column by its identification number. The first letter following that number is the property code--P for vapor pressure, D for liquid density, and B for second virial coefficient. The second is either U for "used" or N for "not used". Those literature documents listed after a U each contributed one data point or more to the selected data base for the correlation. All the data points in documents following an N were excluded from the correlation data base. For each compound, the properties are listed in the order P, B and D. Lines which contain no reference numbers have been deleted in this tabulation. Note that all the literature documents for virial coefficient data follow the U code because those data were not subjected to the selection-deletion process used for the vapor pressure and density.

The citations for the literature documents listed in Table 19 and cited in the text of this report are given in Table 20.

## 9. Acknowledgements

Financial support for this project was provided by the Office of Standard Reference Data and by the Industrial Participants in the Thermodynamics Research Laboratory.

Table 19. Literature references for individual property correlations

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|        |   |   |       |       |       |       |       |       |       |       |       |       |       |
|--------|---|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| KE0300 | P | U | 00709 | 01514 | 02560 | 02575 | 05881 | 07952 | 10044 | 10253 | 10318 | 11081 | 16497 |
| KE0300 | P | U | 41354 | 41545 | 41685 |       |       |       |       |       |       |       |       |
| KE0300 | P | N | 00041 | 00129 | 00130 | 00189 | 00196 | 00202 | 00219 | 00340 | 00721 | 01284 | 01348 |
| KE0300 | P | N | 01359 | 01361 | 01578 | 01638 | 01674 | 01683 | 01780 | 01803 | 01826 | 01880 | 02242 |
| KE0300 | P | N | 02422 | 02478 | 02595 | 02673 | 02894 | 02899 | 02920 | 03087 | 03855 | 04423 | 04455 |
| KE0300 | P | N | 04637 | 04743 | 04839 | 05000 | 05030 | 05067 | 05143 | 05182 | 05901 | 05981 | 06035 |
| KE0300 | P | N | 06102 | 06104 | 06106 | 06108 | 06111 | 06115 | 06119 | 06482 | 06765 | 07073 | 07127 |
| KE0300 | P | N | 07140 | 07406 | 07510 | 07948 | 08672 | 09546 | 09767 | 10037 | 10131 | 10165 | 10358 |
| KE0300 | P | N | 10586 | 10763 | 10830 | 10841 | 10968 | 11019 | 11097 | 11364 | 11373 | 11410 | 11857 |
| KE0300 | P | N | 14102 | 15362 | 15518 | 15521 | 16587 | 16683 | 16911 | 17538 | 18048 | 18275 | 19402 |
| KE0300 | P | N | 19439 | 19951 | 20019 | 20137 | 20426 | 20469 | 20484 | 20711 | 21878 | 22903 | 22906 |
| KE0300 | P | N | 40067 | 40207 | 40217 | 40642 | 40979 | 41162 | 41522 | 41586 | 41759 |       |       |
| KE0300 | D | U | 00709 | 00777 | 01359 | 02478 | 05204 | 09277 | 10165 | 11019 | 15755 | 40228 |       |
| KE0300 | D | N | 00072 | 00852 | 01360 | 02449 | 02509 | 02546 | 02608 | 02962 | 04606 | 04731 | 05857 |
| KE0300 | D | N | 07127 | 07919 | 10163 | 14087 | 14102 | 14146 | 17032 | 19402 | 22860 | 23109 | 40207 |
| KE0300 | D | N | 40489 | 40816 |       |       |       |       |       |       |       |       |       |
| KE0300 | B | U | 01257 | 01803 | 01950 | 02422 | 02678 | 05214 | 05283 | 05948 | 08330 | 08577 | 09027 |
| KE0300 | B | U | 10972 | 20469 |       |       |       |       |       |       |       |       |       |
| KE0305 | P | U | 40217 |       |       |       |       |       |       |       |       |       |       |
| KE0340 | D | U | 13835 |       |       |       |       |       |       |       |       |       |       |
| KE0360 | P | U | 22644 |       |       |       |       |       |       |       |       |       |       |
| KE0360 | P | N | 07198 |       |       |       |       |       |       |       |       |       |       |
| KE0361 | P | U | 22644 |       |       |       |       |       |       |       |       |       |       |
| KE0362 | P | U | 22644 |       |       |       |       |       |       |       |       |       |       |
| KE0370 | P | U | 10015 |       |       |       |       |       |       |       |       |       |       |
| KE0380 | P | U | 07465 | 10015 | 15034 | 16255 | 23080 |       |       |       |       |       |       |
| KE0380 | D | U | 07465 |       |       |       |       |       |       |       |       |       |       |
| KE0380 | D | N | 10015 | 15034 |       |       |       |       |       |       |       |       |       |
| KE0400 | P | U | 00697 | 01005 | 02920 | 03760 | 10318 | 10901 | 11081 |       |       |       |       |
| KE0400 | P | N | 01146 | 01361 | 01780 | 01880 | 01882 | 01985 | 02560 | 03209 | 04418 | 05030 | 05067 |
| KE0400 | P | N | 06128 | 06763 | 07162 | 07439 | 08193 | 08971 | 09712 | 10834 | 10998 | 11017 | 11130 |
| KE0400 | P | N | 11162 | 11178 | 13138 | 13799 | 14102 | 17059 | 20484 | 22466 | 40936 | 41379 |       |
| KE0400 | D | U | 00241 | 01859 | 02045 | 02478 | 02920 | 03386 | 04220 | 06763 | 07452 | 09002 | 09712 |
| KE0400 | D | U | 10163 | 11017 | 11243 | 12590 | 14102 | 15411 | 20486 | 40566 | 40936 | 41379 |       |
| KE0400 | D | N | 00288 | 01360 | 03209 | 03974 | 05076 | 07439 | 07470 | 08860 | 09920 | 10449 | 11072 |
| KE0400 | D | N | 13138 | 14815 | 15755 | 17059 | 17194 | 19999 | 21419 | 23174 | 23353 | 40489 | 41041 |
| KE0400 | B | U | 10901 | 21584 |       |       |       |       |       |       |       |       |       |
| KE0410 | P | U | 01732 | 10537 | 14792 |       |       |       |       |       |       |       |       |
| KE0410 | P | N | 15791 | 19474 |       |       |       |       |       |       |       |       |       |
| KE0420 | P | U | 22762 | 40284 |       |       |       |       |       |       |       |       |       |
| KE0420 | P | N | 03383 | 06237 | 18654 |       |       |       |       |       |       |       |       |
| KE0420 | D | U | 03383 | 06237 | 40284 |       |       |       |       |       |       |       |       |
| KE0420 | D | N | 18654 |       |       |       |       |       |       |       |       |       |       |
| KE0430 | P | U | 13997 |       |       |       |       |       |       |       |       |       |       |
| KE0430 | D | U | 13997 |       |       |       |       |       |       |       |       |       |       |
| KE0440 | P | U | 02219 | 05999 | 10531 | 18774 |       |       |       |       |       |       |       |
| KE0440 | P | N | 15628 |       |       |       |       |       |       |       |       |       |       |
| KE0445 | P | U | 11752 |       |       |       |       |       |       |       |       |       |       |

Table 19. Literature references for individual property correlations--Continued

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KE0445 P N 09754  
 KE0446 P U 22770  
 KE0450 P U 14415  
 KE0451 P U 14415  
 KE0460 P U 15556  
 KE0500 P U 04418 05067 10318 10901  
 KE0500 P N 02314 02369 05143 06717 07406 07439 09920 10560 11097 11733 12038  
 KE0500 P N 13138 13799 21281 40936  
 KE0500 D U 07439 07470 40489  
 KE0500 D N 02369 02456 05759 07372 07483 07611 09002 09712 09920 10483 10560  
 KE0500 D N 11733 12038 13065 13138 15411 20486 40566 40936 41156  
 KE0500 B U 10901  
 KE0501 P U 04033 05067 10318  
 KE0501 P N 00947 01091 01361 03069 03549 04418 05839 06216 07439 07879 10539  
 KE0501 P N 11097 11733 21281 22906  
 KE0501 D U 01360 05839 07483 09920 11733 13138 15411 17509 40353 40425 40566  
 KE0501 D U 41156  
 KE0501 D N 02856 02894 04220 04269 04703 06216 07439 07449 07470 07879 13065  
 KE0501 D N 20615  
 KE0501 B U 04033 21584  
 KE0505 P U 04033 05067 10318  
 KE0505 P N 01091 01361 07406 11733 13799 21601  
 KE0505 D U 01091 21601  
 KE0505 D N 04703 13065 13151  
 KE0505 B U 04033  
 KE0510 P U 15791 16370 41430  
 KE0510 P N 02314 05858 06747 07919 09948 21283  
 KE0510 D U 05858 13839  
 KE0510 D N 02663 03512 06747 13847 15791 16355 22775  
 KE0520 P U 02060 05067 07406 22762 40284  
 KE0520 P N 04670 07948 08193 09754 09923 10472 14204 14453 18654 18956 21047  
 KE0520 P N 21283 21545 22760 40156  
 KE0520 D U 00072 02840 04670 07948 18654 18956 40156  
 KE0520 D N 04269 09923 14204 21198 21388  
 KE0530 P U 13292 15758  
 KE0530 P N 05999 08166 14422 15701  
 KE0530 D U 14422  
 KE0530 D N 05999 13292 15701  
 KE0540 P U 01361 23278  
 KE0540 P N 13151  
 KE0540 D U 01360 23270  
 KE0540 D N 05999 10531 15628 18774  
 KE0555 P U 13274  
 KE0563 P U 01361  
 KE0563 D U 01360  
 KE0565 P U 07045  
 KE0566 P U 01146  
 KE0568 D U 22784  
 KE0570 P U 13274  
 KE0600 P U 10318  
 KE0600 P N 02314 07439 09712 11733 12996 13065 13138 13799 21283

Table 19. Literature references for individual property correlations--Continued

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KE0600 D U 01091 07439 09712 13065  
 KE0600 D N 04703 12996 13138 40489  
 KE0601 P U 04033 10318  
 KE0601 P N 04418 07570 13065 13138 16695 21283  
 KE0601 D U 13065 13138  
 KE0601 D N 07439  
 KE0601 B U 04033  
 KE0604 P U 01091 05067 11773 13065  
 KE0604 P N 00925 01856 03750 06080 07319 08145 08181 08768 09138 11733 13799  
 KE0604 P N 15869 17908 19474 22902 23180 40230 40936 41379  
 KE0604 D U 05115 07470 09138 11733 11773 15411 22902 23180 40228 41379 41407  
 KE0604 D U 41622  
 KE0604 D N 00925 03699 05876 07439 11233 13065 15869 20519 20529 40936  
 KE0605 P U 08181 13065 15776 21544  
 KE0605 P N 13799  
 KE0607 P U 10318 13065  
 KE0607 P N 05876 07301 07406 08193 10483  
 KE0607 D U 10483  
 KE0607 D N 05876 13065 22773  
 KE0610 D U 03512 16355  
 KE0610 D N 09493 14025  
 KE0615 D U 13839  
 KE0620 P U 01095 03023 04670 10697 18421 18956 19429 40158  
 KE0620 P N 02060 02894 04720 06763 08539 08915 09923 10569 14204 14453 15791  
 KE0620 P N 16574 18654 19474 21283 22760 23135 23414 40682  
 KE0620 D U 01529 02840 02894 04670 06763 40158  
 KE0620 D N 02456 04269 04731 09923 11502 14204 15702 15791 18421 18654 18956  
 KE0620 D N 21365 23395  
 KE0625 D U 09923  
 KE0640 P U 05067  
 KE0640 P N 22452  
 KE0645 P U 13236  
 KE0650 P U 11773 13236  
 KE0650 P N 03023 04755 10472 14453 20809 21283  
 KE0650 D U 11773  
 KE0650 D N 01176 13236 20809 22408  
 KE0660 P U 20670  
 KE0660 D U 14192  
 KE0670 P U 01146 06962  
 KE0670 P N 05741 09754 11773 12938  
 KE0670 D U 11773  
 KE0670 D N 20707  
 KE0680 P U 22755  
 KE0700 P U 01499 10318  
 KE0700 P N 07439 10483 12038 13065 14905  
 KE0700 D U 09712 10483 12038  
 KE0700 D N 04269 07439 07470 07601 12996 13065 13138 13155 14905 23251  
 KE0701 D U 07601 14417 23251  
 KE0701 D N 13138  
 KE0702 P U 01091 02314 11733 16695  
 KE0702 P N 03549 03760 04220 07439 07601 11735 13138 13155 14649 18394 19474

Table 19. Literature references for individual property correlations--Continued

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KE0702 P N 19842 20779 21544  
 KE0702 D U 07470 11733  
 KE0702 D N 00182 04220 04269 04703 07439 07601 12628 13138 13155 22773 23251  
 KE0710 P U 13799  
 KE0720 P U 01361 07406 13799  
 KE0720 P N 03069 08161 08181 10472 10483 13065 13155 14649 19474  
 KE0720 D U 10483 13155  
 KE0720 D N 01360 10472 13065 22773  
 KE0725 D U 00182 13846  
 KE0730 D U 13839  
 KE0735 D U 13839  
 KE0740 P U 18654 40284  
 KE0740 P N 09874 09923 14204 14618 21544  
 KE0740 D U 40284  
 KE0740 D N 09923 18654  
 KE0745 D U 09862 09923 14219  
 KE0745 D N 10707  
 KE0746 D U 09923 14219  
 KE0746 D N 09862 14380  
 KE0747 D U 01990 09862 09923 10707 14219  
 KE0747 D N 14380  
 KE0760 D U 14192  
 KE0800 P U 05842 09712 15791 18439  
 KE0800 P N 05736 05846 07439 07448 12996 18392 18716 19474 21283 21544  
 KE0800 D U 05736 05846 07470 19380 40489  
 KE0800 D N 05842 07439 07449 09712 12996 18439 22773  
 KE0801 P U 13138 14417 18439  
 KE0801 P N 07570  
 KE0801 D U 13138 14417  
 KE0801 D N 18439  
 KE0802 P U 18439  
 KE0802 P N 13138  
 KE0802 D U 13138  
 KE0802 D N 18439  
 KE0810 P U 13799  
 KE0830 P U 13799  
 KE0850 P U 01146  
 KE0850 P N 07301 19474 23310  
 KE0850 D U 21602  
 KE0870 P U 13799  
 KE0870 P N 08193  
 KE0890 P U 40284  
 KE0890 P N 09874 14712 18654  
 KE0890 D U 40284  
 KE0910 P U 09717  
 KE0910 D U 09717  
 KE0930 D U 13846  
 KE0950 P U 01176 02475 04651 05772 10722 11049 18392 20809  
 KE0950 P N 03023 04217 07449 08193 10579 14417 14464 14697 15698 17061  
 KE0950 D U 02475 07372 11049 12707 14417 15698 17061 20809 40489 40688  
 KE0950 D N 00182 04269 04569 07449 13407 13566 19928

Table 19. Literature references for  
individual property correlations--Continued

|        |   |   |       |                         |
|--------|---|---|-------|-------------------------|
| KE0980 | P | U | 01361 |                         |
| KE0980 | D | U | 01360 |                         |
| KE1000 | P | U | 05736 | 12038                   |
| KE1000 | P | N | 06109 | 09712 14417             |
| KE1000 | D | U | 09712 | 12038                   |
| KE1000 | D | N | 05736 | 14417                   |
| KE1001 | D | U | 14417 |                         |
| KE1002 | D | U | 13138 |                         |
| KE1003 | P | U | 10318 |                         |
| KE1003 | P | N | 01711 | 03549 13138 14417 14649 |
| KE1003 | D | U | 01091 | 13138 14417             |
| KE1003 | D | N | 01631 | 11733                   |
| KE1020 | P | U | 05775 |                         |
| KE1020 | P | N | 01856 | 07439 21283             |
| KE1020 | D | U | 05775 | 07439                   |
| KE1020 | D | N | 41661 |                         |
| KE1040 | D | U | 21602 |                         |
| KE1060 | P | U | 13799 |                         |
| KE1100 | P | U | 18654 |                         |
| KE1100 | P | N | 09874 |                         |
| KE1150 | D | U | 14195 |                         |
| KE1150 | D | N | 20774 | 22408                   |
| KE1180 | P | U | 01361 | 03396 18395             |
| KE1180 | P | N | 05988 | 07288 13438 14417       |
| KE1180 | D | U | 14417 |                         |
| KE1180 | D | N | 00182 | 01360 03512 13407 40489 |
| KE1181 | D | U | 14417 | 40688 41319             |
| KE1181 | D | N | 18601 |                         |
| KE1200 | P | U | 06619 | 14453                   |
| KE1200 | P | N | 13438 | 14464 18717 21283 22680 |
| KE1250 | D | U | 00182 |                         |
| KE1250 | D | N | 05988 |                         |
| KE1320 | D | U | 06921 |                         |
| KE1350 | D | U | 14195 |                         |
| KE1360 | D | U | 14195 |                         |
| KE1400 | D | U | 09712 | 21072                   |
| KE1401 | D | U | 14417 |                         |
| KE1403 | D | U | 13138 |                         |
| KE1403 | D | N | 07296 |                         |
| KE1500 | P | U | 18654 |                         |
| KE1500 | P | N | 09874 |                         |
| KE1530 | D | U | 13811 |                         |
| KE1530 | D | N | 10887 | 14382                   |
| KE1550 | D | U | 06837 |                         |
| KE1580 | D | U | 09923 | 14204                   |
| KE1600 | P | U | 06619 |                         |
| KE1600 | P | N | 01856 | 19474 21283             |
| KE1620 | P | U | 21109 | 21948                   |
| KE1620 | P | N | 03513 | 05143 05865             |
| KE1620 | D | U | 12455 |                         |
| KE1640 | D | U | 06237 | 20930                   |

Table 19. Literature references for  
individual property correlations--Continued

|        |   |   |       |       |       |       |       |       |       |
|--------|---|---|-------|-------|-------|-------|-------|-------|-------|
| KE1660 | D | U | 20809 |       |       |       |       |       |       |
| KE1680 | D | U | 20809 |       |       |       |       |       |       |
| KE1700 | P | U | 06619 |       |       |       |       |       |       |
| KE1700 | P | N | 07198 | 18395 | 19474 |       |       |       |       |
| KE1720 | P | U | 08739 | 15685 |       |       |       |       |       |
| KE1750 | D | U | 05988 | 14417 | 40489 |       |       |       |       |
| KE1750 | D | N | 07449 | 13407 |       |       |       |       |       |
| KE1760 | D | U | 14417 |       |       |       |       |       |       |
| KE1762 | D | U | 14417 | 40688 |       |       |       |       |       |
| KE1762 | D | N | 18601 |       |       |       |       |       |       |
| KE1800 | P | U | 13305 |       |       |       |       |       |       |
| KE1820 | P | U | 10983 |       |       |       |       |       |       |
| KE1821 | P | U | 10983 |       |       |       |       |       |       |
| KE1860 | D | U | 13839 |       |       |       |       |       |       |
| KE1900 | P | U | 11006 |       |       |       |       |       |       |
| KE1901 | P | U | 11006 |       |       |       |       |       |       |
| KE2000 | D | U | 14195 |       |       |       |       |       |       |
| KE2100 | P | U | 10318 | 12038 |       |       |       |       |       |
| KE2100 | P | N | 05746 | 08131 | 08465 | 09712 | 10483 | 14417 | 19474 |
| KE2100 | D | U | 10483 | 12038 |       |       |       |       |       |
| KE2100 | D | N | 08465 | 09712 | 14417 |       |       |       |       |
| KE2104 | P | U | 10318 | 13138 |       |       |       |       |       |
| KE2104 | P | N | 14003 | 14417 | 14649 | 20317 |       |       |       |
| KE2104 | D | U | 13138 | 14417 |       |       |       |       |       |
| KE2104 | D | N | 22773 |       |       |       |       |       |       |
| KE2120 | P | U | 40284 |       |       |       |       |       |       |
| KE2120 | P | N | 18654 |       |       |       |       |       |       |
| KE2120 | D | U | 40284 |       |       |       |       |       |       |
| KE2120 | D | N | 18654 |       |       |       |       |       |       |
| KE2130 | D | U | 14195 |       |       |       |       |       |       |
| KE2150 | D | U | 06711 | 13407 | 40489 |       |       |       |       |
| KE2155 | D | U | 14417 |       |       |       |       |       |       |
| KE2170 | D | U | 05988 |       |       |       |       |       |       |
| KE2190 | D | U | 14195 |       |       |       |       |       |       |
| KE2225 | P | U | 40284 |       |       |       |       |       |       |
| KE2225 | P | N | 18654 |       |       |       |       |       |       |
| KE2225 | D | U | 40284 |       |       |       |       |       |       |
| KE2235 | D | U | 06837 |       |       |       |       |       |       |
| KE2250 | D | U | 06711 |       |       |       |       |       |       |
| KE2250 | D | N | 13407 | 18400 |       |       |       |       |       |
| KE2260 | D | U | 14713 |       |       |       |       |       |       |
| KE2261 | P | U | 04651 |       |       |       |       |       |       |
| KE2300 | P | U | 10318 | 12038 |       |       |       |       |       |
| KE2300 | P | N | 08131 | 09712 |       |       |       |       |       |
| KE2300 | D | U | 12038 |       |       |       |       |       |       |
| KE2300 | D | N | 09712 |       |       |       |       |       |       |
| KE2330 | P | U | 01146 | 05725 | 20809 |       |       |       |       |
| KE2331 | P | U | 05725 |       |       |       |       |       |       |
| KE2350 | D | U | 06711 |       |       |       |       |       |       |
| KE2350 | D | N | 13407 |       |       |       |       |       |       |
| KE2365 | P | U | 01361 | 04651 | 06664 | 07481 | 40222 |       |       |

Table 19. Literature references for individual property correlations--Continued

|        |   |   |       |       |       |       |       |       |       |       |       |       |
|--------|---|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| KE2365 | P | N | 05725 | 08227 | 15340 | 15341 | 15698 | 17342 | 19962 | 20007 | 20318 | 20811 |
| KE2365 | D | U | 00182 |       | 20318 |       |       |       |       |       |       |       |
| KE2365 | D | N | 05990 | 07372 | 07919 | 15698 |       |       |       |       |       |       |
| KE2380 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE2430 | D | U | 14192 |       |       |       |       |       |       |       |       |       |
| KE2445 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE2460 | P | U | 06817 | 17342 |       |       |       |       |       |       |       |       |
| KE2460 | D | U | 20318 |       |       |       |       |       |       |       |       |       |
| KE2473 | P | U | 11052 |       |       |       |       |       |       |       |       |       |
| KE2474 | P | U | 10550 |       |       |       |       |       |       |       |       |       |
| KE2477 | P | U | 10550 |       |       |       |       |       |       |       |       |       |
| KE2506 | P | U | 10318 |       |       |       |       |       |       |       |       |       |
| KE2506 | P | N | 05736 | 08131 |       |       |       |       |       |       |       |       |
| KE2506 | D | U | 14905 | 19014 |       |       |       |       |       |       |       |       |
| KE2540 | D | U | 06711 |       |       |       |       |       |       |       |       |       |
| KE2540 | D | N | 13407 |       |       |       |       |       |       |       |       |       |
| KE2545 | P | U | 13834 |       |       |       |       |       |       |       |       |       |
| KE2545 | P | N | 08166 |       |       |       |       |       |       |       |       |       |
| KE2565 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE2630 | D | U | 14195 |       |       |       |       |       |       |       |       |       |
| KE2645 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE2680 | D | U | 14195 |       |       |       |       |       |       |       |       |       |
| KE2685 | D | U | 14195 |       |       |       |       |       |       |       |       |       |
| KE2688 | D | U | 14195 |       |       |       |       |       |       |       |       |       |
| KE2707 | D | U | 14905 |       |       |       |       |       |       |       |       |       |
| KE2745 | D | U | 14195 |       |       |       |       |       |       |       |       |       |
| KE2755 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE2775 | P | U | 11052 |       |       |       |       |       |       |       |       |       |
| KE2835 | D | U | 06711 |       |       |       |       |       |       |       |       |       |
| KE2845 | D | U | 14713 |       |       |       |       |       |       |       |       |       |
| KE3050 | D | U | 06711 |       |       |       |       |       |       |       |       |       |
| KE3310 | D | U | 19014 |       |       |       |       |       |       |       |       |       |
| KE3350 | P | U | 08226 |       |       |       |       |       |       |       |       |       |
| KE3350 | P | N | 06753 |       |       |       |       |       |       |       |       |       |
| KE3350 | D | U | 08125 |       |       |       |       |       |       |       |       |       |
| KE3712 | D | U | 19014 |       |       |       |       |       |       |       |       |       |
| KE4114 | D | U | 08125 |       |       |       |       |       |       |       |       |       |
| KE4114 | D | N | 19014 |       |       |       |       |       |       |       |       |       |

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